REPORT DOCUMENTATION PAGE	Form Approved OMB NO. 0704-0188

1. REPORT DATE (DD-MM-YYYY) 21-08-2015	2. REPORT TYPE Final Report	3. DATES COVERED (From - To) 1-Oct-2011 - 31-Mar-2015

4. TITLE AND SUBTITLE Final Report: Autoignition Chemistry of Surrogate Fuel Components in an Engine Environment	5a. CONTRACT NUMBER W911NF-11-1-0412
	5b. GRANT NUMBER
	5c. PROGRAM ELEMENT NUMBER 611102
6. AUTHORS David L Miller, Nicholas P Cernansky	5d. PROJECT NUMBER
	5e. TASK NUMBER
	5f. WORK UNIT NUMBER

7. PERFORMING ORGANIZATION NAMES AND ADDRESSES Drexel University Office of Research 3201 Arch Street, Suite 100 Philadelphia, PA 19104 -2875	8. PERFORMING ORGANIZATION REPORT NUMBER

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS (ES) U.S. Army Research Office P.O. Box 12211 Research Triangle Park, NC 27709-2211	10. SPONSOR/MONITOR'S ACRONYM(S) ARO
	11. SPONSOR/MONITOR'S REPORT NUMBER(S) 59135-EG.1

12. DISTRIBUTION AVAILIBILITY STATEMENT

Approved for Public Release; Distribution Unlimited

13. SUPPLEMENTARY NOTES
The views, opinions and/or findings contained in this report are those of the author(s) and should not contrued as an official Department of the Army position, policy or decision, unless so designated by other documentation.

14. ABSTRACT
This is the final report of a program to investigate the autoignition behavior and chemistry of JP-8 components and blends in a single-cylinder, variable compression ratio research engine. The program objectives were to determine the branching pathways of JP-8 components at autoignition conditions; establish the impact of recycle fraction on chemistry, and aid in the development of chemical models. The program has made progress toward making the measurements that will resolve these issues. The study has mapped the reactivity of components in present and future JP-8 type fuels as a basis for beginning the studies of gas sampling from the exhaust and in-cylinder which

15. SUBJECT TERMS
Hydrocarbon Oxidation in Engines; Hydrocarbon Autognition in Engines; Next Generation Fuels; Surrogate Fuels

16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	15. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON David Miller
a. REPORT UU	b. ABSTRACT UU	c. THIS PAGE UU	UU		19b. TELEPHONE NUMBER 215-895-2429

Report Title

Final Report: Autoignition Chemistry of Surrogate Fuel Components in an Engine Environment

ABSTRACT

This is the final report of a program to investigate the autoignition behavior and chemistry of JP-8 components and blends in a single-cylinder, variable compression ratio research engine. The program objectives were to determine the branching pathways of JP-8 components at autoignition conditions; establish the impact of recycle fraction on chemistry, and aid in the development of chemical models. The program has made progress toward making the measurements that will resolve these issues. The study has mapped the reactivity of components in present and future JP-8 type fuels as a basis for beginning the studies of gas sampling from the exhaust and in-cylinder which will aid in identifying reaction pathways. The work has also proposed a new way to compare the reactivity of hydrocarbons. However, the initial updating of the facility and the required relocation, occurring during the third year, took more time than expected and consequently, we were unable to fully achieve the program objectives. The PI's are committed to continuing the work with in-house funding promised as compensation for the lost time during the relocation. Results of this ongoing work will acknowledge the support of ARO and resulting dissertations and manuscripts will be submitted to the ARO archives.

Enter List of papers submitted or published that acknowledge ARO support from the start of the project to the date of this printing. List the papers, including journal references, in the following categories:

(a) Papers published in peer-reviewed journals (N/A for none)

<u>Received</u>   <u>Paper</u>

TOTAL:

Number of Papers published in peer-reviewed journals:

(b) Papers published in non-peer-reviewed journals (N/A for none)

<u>Received</u>   <u>Paper</u>

TOTAL:

Number of Papers published in non peer-reviewed journals:

(c) Presentations

Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

<u>Received</u>   <u>Paper</u>

TOTAL:

Number of Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Peer-Reviewed Conference Proceeding publications (other than abstracts):

<u>Received</u>   <u>Paper</u>

TOTAL:

Number of Peer-Reviewed Conference Proceeding publications (other than abstracts):

(d) Manuscripts

<u>Received</u>   <u>Paper</u>

TOTAL:

Number of Manuscripts:

Books

<u>Received</u>   <u>Book</u>

  TOTAL:

<u>Received</u>   <u>Book Chapter</u>

  TOTAL:

Patents Submitted

Patents Awarded

Awards

NA

Graduate Students

NAME	PERCENT_SUPPORTED	Discipline
Yulei Li	1.00	
MIchael Stichter	0.25	
FTE Equivalent:	**1.25**	
Total Number:	**2**	

Names of Post Doctorates

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Names of Faculty Supported

NAME	PERCENT_SUPPORTED	National Academy Member
David L Miller	0.05	
Nicholas P Cernansky	0.05	
FTE Equivalent:	**0.10**	
Total Number:	**2**	

Names of Under Graduate students supported

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Student Metrics
This section only applies to graduating undergraduates supported by this agreement in this reporting period

The number of undergraduates funded by this agreement who graduated during this period: 0.00

The number of undergraduates funded by this agreement who graduated during this period with a degree in science, mathematics, engineering, or technology fields:...... 0.00

The number of undergraduates funded by your agreement who graduated during this period and will continue to pursue a graduate or Ph.D. degree in science, mathematics, engineering, or technology fields:...... 0.00

Number of graduating undergraduates who achieved a 3.5 GPA to 4.0 (4.0 max scale):...... 0.00

Number of graduating undergraduates funded by a DoD funded Center of Excellence grant for Education, Research and Engineering:...... 0.00

The number of undergraduates funded by your agreement who graduated during this period and intend to work for the Department of Defense 0.00

The number of undergraduates funded by your agreement who graduated during this period and will receive scholarships or fellowships for further studies in science, mathematics, engineering or technology fields:...... 0.00

Names of Personnel receiving masters degrees

NAME
Total Number:

Names of personnel receiving PHDs

NAME
Total Number:

Names of other research staff

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Sub Contractors (DD882)

Inventions (DD882)

Scientific Progress

See Attachment

Technology Transfer

Discussions have occurred within the community of researchers (academic, industrial, government laboratories) on next generation fuels and engines at professional meetings, such as Combustion Institute Conferences, SAE International Congress, etc.

Autoignition Chemistry of Surrogate Fuel Components in an Engine Environment

David L. Miller and Nicholas P. Cernansky

Mechanical Engineering and Mechanics

Drexel University, Philadelphia, Pennsylvania, 19104

Objective

The program investigated the autoignition behavior and chemistry of JP-8 surrogate components and blends in a single-cylinder research engine. Alkanes, cycloalkanes and alkylated aromatic hydrocarbons relevant to JP-8 and surrogate blends were to be examined. Analysis of these results and continued work were to be used for: (1) determination of the key branching pathways of these JP-8 surrogates at autoignition conditions; (2) establishing the impact on chemistry of recycle fraction in engines; and (3) development of the next generation of JP-8 surrogates and chemical models.

Approach

The reactivity of selected alkanes, cycloalkanes, and alkylated aromatics relevant to JP-8 and surrogate blends was to be examined in a motored engine with variable compression ratio. Initially, in-cylinder pressure traces were measured while varying parameters such as equivalence ratio, engine speed, and manifold inlet temperature and pressure in order to identify reactivity regimes for selected hydrocarbons. Changes in compression ratio and inlet pressure change the percentages of trapped residuals and should allow exploration of their impact on reactivity. Exhaust and in-cylinder gas composition were to be analyzed to identify the intermediate species produced and to generate species profiles as function of reaction conditions.

Relevance to Army

Research on combustion in CI engines is an important need for Army ground transportation systems, including fundamental research on low temperature physical and chemical rate processes and on developing appropriate surrogates for JP-8 (as the 'single fuel forward') for future engine development. The research will contribute to both of these areas by: (1) determining the key branching pathways of selected JP-8 surrogate components at engine conditions leading to ignition; (2) establishing the connection between the engine experiments and more fundamental experimental systems; and (3) assisting in the development of the next generation of JP-8 surrogates. In general, speciation data during the pre-ignition of JP-8 is presently scarce, so additional studies using higher molecular weight fuels and fuel components will provide useful, new information. Ultimately, this research will aid the Army as it moves to optimize the use of JP-8 as the single fuel forward in all reciprocating engines. – improving efficiencies and power density.

Accomplishments for the Project

The research was carried out in the Combustion Chemistry Laboratory of the Mechanical Engineering and Mechanics Department at Drexel University, and utilized an existing single cylinder research engine facility. The facility, schematic shown in Fig. 1, consists of a modified CFR (Cooperative Fuel Research) engine coupled to a dynamometer. In practical compression

ignition engines, auto-ignition occurs in the premixed spray envelope that forms during the fuel injection process. To focus on this regime without the complications of spray and mixing transients, a fully pre-vaporized and premixed intake condition is utilized in the present study. To achieve this, fuels are injected into the air stream of a heated inlet manifold well upstream of the intake valve to assure complete vaporization and mixing. A key feature of this engine is a movable cylinder head that allows variation of the compression ratio from 4:1 to 18:1. The bore is 0.0825 m, the stroke is 0.1143 m, and the displacement is 6.116×10^{-4} m^3. The standard intake valve opening, intake valve closing, exhaust valve opening, and exhaust valve closing are 10 bTDC, 34 aBDC, 40 bBDC, and 15 aTDC, respectively, where TDC represents the piston at the top position, BDC is the piston at the bottom position, and a and b are after and before. The valve timing can be adjusted to vary the residual fraction by employing a variable valve actuation system as demonstrated by Zheng et al., 2003. A pressure transducer inside the cylinder measures the in-cylinder pressure, and a shaft encoder monitors the crankshaft position, recorded as crank angle degrees (CAD), with uncertainties of ±0.2 CAD. Motored operation at 16:1 CR with inlet conditions of 25 C and 1 bar results in TDC conditions of ~1000 K and 25 Bar.

YEAR 01

As the program began, it became obvious that several of the engine systems were not operating properly. In particular, the data acquisition system required a redesign of both the hardware and software. During initial shakedown experiments the pressure transducer was identified as only partially functional and that also required replacement. After resolving these issues it was decided to plan a set of initial experiments that let us define a baseline of engine performance and validate the operation of the engine test facility.

In the first set of baseline experiments, the engine was operated with only air as the in-cylinder charge at the range of conditions planned for the program. The conditions projected to be used during the initial phases of the study are compression ratio (CR) of 5.5 to 8.5; intake temperature (IT) 350-450 K; and fuel to air equivalence ratio (ER) of 0.2-0.3. Figure 2 presents the results of these experiments. The traces are smooth, symmetrical about compression top dead center (Crank angle = 360) and show the expected trends of increasing maximum pressure with increasing IT or increasing CR.

It is interesting to note the difference in the profiles for the same sweep in IT and CR with the air charge as opposed to a fuel charge of n-heptane at an ER of 0.3 (Fig. 3). N-heptane was selected as it has been previously studied and would provide a set of experiments to validate the performance of the updated engine. It is also a representative straight chain component of a JP-8 surrogate. Heat release from the partial oxidation of the fuel produces a marked increase in pressure. The shape and phasing of this profile changes based on the interaction of the temperature versus crank angle history produced by the differing compression ratios and the fuels relative reactivity at those temperatures. For low compression ratios, which produce lower in-cylinder temperatures the reactivity is delayed and is less intense, producing an increase in pressure above the air trace after TDC and a relatively mild increase in pressure of 10%. For higher compression ratios the deviation begins earlier in the cycle and can be as much as 200%. For this hydrocarbon alkane the behavior of is further complicated by the appearance of a two-stage deviation from the air profile produced by the manifestation of negative temperature coefficient (NTC) reactivity that is characteristic of alkanes. During this NTC behavior the reactivity of the fuel actually decreases as the temperature increases

To further explore the effect of ER on the reactivity two sets of experiments were performed changing ER from 0.2 to 0.3, fixing the IT at 350, 400, and 450K, and operating at either CR=7 (Fig. 4) or CR=8.5 (Fig. 5). At low ER (very lean conditions) the pressure traces are very similar to the results for the air conditions with minimal deviation until well after TDC and then primarily at the higher intake temperatures. At ER=0.3, the pressure traces show strong two-stage reactivity which commences well before TDC and produces the large pressures of fuel autoignition.

It is also interesting to examine the data for fixed ER and CR for the three intake temperatures (ITs) of the study (Fig. 6). For the lower CR of 7.0 the effect of inlet temperature is non-intuitive. At the lowest IT the phasing of the first stage heat release and the primary heat release occurring after TDC produces a maximum pressure of 25 bar; while at the intermediate temperature first stage reactivity produces heat release beginning before TDC but the fuel charge enters its negative coefficient region and a more gradual reaction proceeds such that the maximum pressure is only 20 bar. For the highest IT, the first stage reactivity is similar to the intermediate case; however the second stage ignitions occurs abruptly before TDC producing a pressure of 25 bar. For the CR=8.5, the fuel charge exhibits two stage ignition at all of the ITs. Due to the timing of the two stages (the first stage reactivity begins closer to TDE) the peak cylinder pressure also occurs for the lowest IT.

Key accomplishments of Year 01 were:
Updated the engine facility
Benchmarked engine performance with n-heptane
Initial mapping of engine conditions necessary to explore effects of ER, IT, and recycle fraction on reactivity that controls autoignition. These experiments demonstrated the complexity of hydrocarbon reactivity in an engine.

YEAR 02
A series of experiments with the possible surrogate components n-decane and n-dodecane were conducted to explore the effect of intake temperature (IT), equivalence ratio (ER) and compression ratio (CR) on auto ignition of these alkanes by acquiring the data of pressure and calculating the temperature in engine chamber. The data showed that both hydrocarbons reacted with two-stage ignition indicative of the negative temperature coefficient (NTC) behavior. For n-decane the conditions of IT, ER, and CR which produced "engine knock" were also mapped. In addition to this, the point when the first stage of ignition happened but the second stage of ignition didn't happen during oxidation of decane in engine was defined. These conditions were also mapped for n-dodecane. This mapping is necessary to select conditions for exhaust gas and possibly in-cylinder sampling in order to pursue the next stage of the study to identify the key reaction pathways controlling ignition in the engine.

In the first set of experiments, the engine was operated with n-dodecane as the in-cylinder charge at CR ranging from 5.5 to 8.5; IT: 400 to 450K, and ER: 0.2 to 0.3. Figure 7 shows the pressure and temperature trace in the engine chamber at condition of ER=0.3, CR=6.3, IT= 600K. Both the pressure and temperature shows the two stage ignition combustion of n-dodecane. The temperature trace shows that the first stage ignition occurred between CAD of 332 to CAD of 341 and the second stage ignition started from CAD of 353. Between these two ignitions the NTC reactivity controls the reactivity, during this NTC behavior the reactivity of the fuel actually decreases as the temperature increases. Figure 8 shows the effect of varying CR. As the CR increased, the maximum value of both pressure and temperature increased. The maximum temperature during combustion reached about 900K. It is interesting to note that at the lowest CR

only a single stage ignition occurred, because the temperature increase caused by compression before TDC was insufficient to trigger the first stage ignition and the entire ignition occurred at TDC. As the CR increased, the compression raised the temperature enough to trigger a first stage ignition and heat release which raised the charge temperature into the NTC region and with further compression into the second stage ignition regime.

The effect of ER on the reactivity was explored with two sets of experiments varying ER from 0.3 to 0.4, while fixing the IT at 400K and CR=6.3. At low ER the pressure and calculated temperature traces show minimal deviation until well after TDC, Fig. 9. Adversely, the pressure and temperature traces at ER=0.4 show strong two-stage reactivity which commences well before TDC and produces the large pressure and temperature of fuel autoignition. Figure 10 shows the effect of varying inlet temperature from 400K to 450K fixing ER=0.3 and CR=6.3. The data show that the fuel charge exhibits two stage ignition at both of the ITs. At the lower IT the phasing of the first stage heat release and the primary heat release occurs after TDC produces a maximum pressure of 16 bar and maximum temperature of 1050K; While at the higher IT the first stage reactivity produces heat release beginning before TDC and the second stage ignitions occurs abruptly before TDC producing a maximum pressure of 19 bar and maximum temperature of 1300 K. As the IT increased, the maximum value of pressure increased.

After the set experiments using n-dodecane, the autoignition of n-decane was explored over a similar range of experimental conditions. The n-decane also showed two-stage ignition. Similarly, higher maximum value of pressure and temperature were reached by higher CR, ER and IT from Figures 11-14. Figure 15 shows the pressure traces of engine chamber when the engine was knocking with the fixing ER of 0.4 and IT of 450K. The pressure traces show the "ringing" that denotes knocking conditions. Different from normal two stage ignition, when the engine was knocking, the pressure raised rapidly, and then kept fluctuating. As CR increased, the fluctuations had higher amplitudes. This sweep of experiments allowed identification of the limiting conditions as the program proceeds to measure species compositions to develop insight into the reaction pathways controlling autoignition in compression ignition engines.

These experiments identify how critical the parameters of ER and IT are to the hydrocarbon reactivity and autoignition. According the Fig. 8, the pressure trace shows one stage ignition for CR as 5.5, the pressure trace shows two stage ignition for CR 6.3. So there must be a critical CR value for fixing ER=03 and IT=400K where only the first stage ignition occurred entirely without second stage ignition

Key accomplishments of Year 02 were:
  Mapping of preignition reactivity from n-decane for selected conditions of ER and IT.
  Mapping of preignition reactivity from n-dodecane for selected conditions of ER and IT.

YEAR 03

During Year 03, the experimental facility was relocated to laboratory in a different building. This move produced a disruption in the program timeline as there was a wait on the installation of some laboratory infrastructure, before the team was able to proceed with equipment recalibration and verification of baseline performance. In order to shorten the downtime an additional graduate student was supported part time.

When the facility came back on line, a new a series of experiments with the possible surrogate components methyl cyclohexane and n-butyl cyclohexane were conducted to explore the effect of intake temperature (IT), equivalence ratio (ER) and compression ratio (CR) on auto ignition of these cycloparaffins by acquiring the data of pressure and calculating the temperature in engine

chamber. The data showed that methyl cyclohexane reacted with two-stage ignition indicative of the negative temperature coefficient (NTC) behavior. N-butyl cyclohexane showed one-stage ignition behavior. In addition to this, the point when the first stage of ignition happened but the second stage of ignition didn't happen during oxidation of methyl cyclohexane in engine was defined.

In the first set of experiments, the engine was operated with methyl cyclohexane as the in-cylinder charge at CR ranging from 10.0 to 12.3; IT: 450 to 500K, and ER: 0.6 to 0.74. Figure 16 shows the pressure and temperature trace in engine chamber at condition of ER=0.72, CR=11.0, IT= 450K. Both the pressure and temperature shows the two stage ignition combustion of methyl cyclohexane. The temperature trace shows that the first stage ignition occurred between CAD of 327 to CAD of 354 and the second stage ignition started from CAD of 363. Between these two ignitions the NTC reactivity controls the reactivity, during this NTC behavior the reactivity of the fuel actually decreases as the temperature increases. Figure 17 shows the effect of varying CR. As the CR increased, the maximum value of both pressure and temperature increased. The maximum temperature during combustion reached about 1780K. It is interesting to note that at the CR=10.5, only a single stage ignition occurred, because the temperature increase caused by compression before TDC was insufficient to trigger the first stage ignition and the entire ignition occurred at TDC. As the CR increased, the compression raised the temperature enough to trigger a first stage ignition and heat release which raised the charge temperature into the NTC region and with further compression into the second stage ignition regime.

To further explore the effect of ER on the reactivity, sets of experiments were carried out varying ER from 0.6 to 0.74, fixing the IT at 450K and CR=11.0, Fig. 18. At low ER the pressure and temperature traces show minimal deviation until well after TDC. Adversely, the pressure and temperature traces at ER=0.74 show strong two-stage reactivity which commences well before TDC and produces the large pressure and temperature of fuel autoignition. Figure 19 shows the effect of varying inlet temperature from 450K to 500K fixing ER=0.72 and CR=11.0. The data show that the fuel charge exhibits two stage ignition at both of the ITs. At the lower IT the primary heat release occurs after TDC produces a maximum pressure of 24 bar and maximum temperature of 1350K; While at the higher IT the first stage reactivity produces heat release beginning before TDC and the second stage ignitions occurs abruptly before TDC producing a maximum pressure of 36 bar and maximum temperature of 2000K. As the IT increased, the maximum value of pressure increased.

After the set experiments using methyl cyclohexane, the autoignition of n-butyl cyclohexane was explored over a similar range of experimental conditions. The n-butyl cyclohexane showed one-stage ignition. Higher maximum value of pressure and temperature were reached by higher CR, ER and IT from Figs. 20-23. It is interesting to note that the fixing ER we set for n-butyl cyclohexane is 0.5. That's because compared with methyl cyclohexane, n-butyl cyclohexane is much more reactive; we have to set lower ER for n-butyl cyclohexane to avoid knocking in the engine.

These experiments have shown the complexity of cycloparaffins reactivity. According to the Fig. 3, note the pressure trace shows one stage ignition for CR of 10.5, the pressure trace shows two stage ignition for CR 11.0. So there must be a critical CR value for fixing ER=0.72 and IT=450K where only the first stage ignition occurred entirely without second stage ignition occurred. In the future work, analytical measurements of exhaust CO with exhaust recycle, monitoring the CO online and measuring intermediate and product species during the running of engine will be performed to find the key reaction pathways at engine condition. After these tasks,

the program will move to experiments on autoignition of selected JP'8 and candidate surrogate mixtures for JP-8. These mixtures will be defined based on analysis of the existing suggestions for JP-8 surrogates.

Key accomplishments of Year 03 were:
Successfully relocated the laboratory.
Mapping of preignition reactivity from methyl cyclohexane for selected conditions of ER and IT.
Mapping of preignition reactivity from butyl cyclohexane for selected conditions of ER and IT.

No-Cost Extension

Experiments explored the effect of intake temperature (IT) and compression ratio (CR) on the auto-ignition of decane. Crank angle resolved cylinder pressure data was acquired and analyzed using an engine heat release code to calculate the associated bulk gas temperature and heat release rate and accumulation. These data showed that decane reacted with two-stage ignition indicative of the negative temperature coefficient (NTC) behavior. In addition, the start of first and second stage of ignition was identified by the heat release profile. The in-cylinder temperature and pressure where these ignition stages occur as engine parameters are varied can be mapped and compared. This allows identification of conditions for exhaust gas and possibly in-cylinder sampling in order to pursue the next phase of the study, which is to identify the key reaction pathways controlling ignition in the engine.

In the present set of mapping experiments with decane, the engine was operated at CR ranging from 6.6 to 7.4; IT from 420 to 440 K, and ER of 0.2. Figure 24 shows the pressure and temperature trace in engine combustion chamber at condition of ER=0.2, CR=7.4, IT=420 K. Both the pressure and temperature shows the two stage ignition combustion of decane. Figure 25 shows the heat release per crank angle degree and the accumulated heat release. The heat release profiles show that the first stage ignition started at CAD of 327 and the second stage ignition started at CAD of 342. Between these two ignition points the NTC chemistry controls the reactivity, and in this NTC region the reactivity of the fuel actually decreases as the temperature increases. According to the Fig. 24, the temperature and pressure when first stage ignition occurs is 610 K and 7.48 Bar.

Figure 26 shows the effect of varying inlet temperature from 420 to 440 K while fixing ER=0.2 and CR=7.4. The data show that the fuel charge exhibits two stage ignition at all ITs, and the 10 K difference of IT doesn't cause too much difference for the pressure profile. However, as the IT increased, the maximum value of temperature in engine chamber increased as well. Fig. 27 shows the heat release profiles as the inlet temperature is varied from 420 to 440 K. We can notice that the general shape of the heat release profile for the oxidation of decane does not vary much with the increase in IT. However, as the IT increased, both the first stage ignition and hot ignition occurred earlier, as expected.

Figure 28 shows the effect of varying CR from 6.6 to 7.4. As the CR increased, the maximum values of both pressure and temperature increased. The maximum temperature during combustion reached about 1260 K at CR of 7.4 as compared to 1100 K at CR of 6.6. Figure 29 shows the heat release profiles with varying CR. At the higher CR of 7.4, the maximum heat release rate is 20 J/CAD, much higher than 10 J/CAD observed with CR of 6.6. Additionally, both the first stage ignition and the hot ignition were advanced with increasing CR, because the temperature and pressure conditions needed for ignition are reached at an earlier crank angle position.

The temperature and pressure conditions when first stage ignition occurred can be determined from the heat release profiles. Figure 30 shows such temperature and pressure conditions for the different ITs. With increasing IT, the pressure at first stage ignition decreases (primarily due to the earlier start of ignition), while the temperature at first stage ignition increases. The line connecting these points is the limit line for the first stage ignition. When more data are available, the limit line for hot ignition can be plotted in the same figure.

Further experiments will be conducted to explore the effect of additional engine parameters, including higher CR and residual gas fraction, on the limit line of first stage ignition and hot ignition. In the future work, analytical measurements of exhaust CO, monitoring the CO online and measuring stable intermediate and product species during the running of engine by GC/MS will be performed to find the key reaction pathways at engine condition.

Key accomplishments through No-cost Extension were:
- Incorporated heat release computations into our analysis to improve locating the first and second stages of heat release.
- Mapping of in-cylinder P and T as a tool to compare critical conditions for first stage ignition. This should provide a way to compare the reactivity of hydrocarbons selected for the study.

Conclusion

The program has made progress toward making the measurements that will yield an answer to the questions raised in the proposal. The study has mapped the reactivity of hydrocarbons that represent the classes of components in present and future JP-8 type fuels as a basis for beginning the studies of gas sampling from the exhaust and perhaps in-cylinder. The work has also proposed a way to compare the reactivity of selected hydrocarbons. However, the initial updating of the facility and the required relocation took much more time than expected and consequently, we were not able to fully achieve the program objectives. The PI's are committed to continuing the work with in-house funding promised as compensation for the lost time during the relocation period of YEAR 03. Results of this ongoing work will acknowledge the support of ARO and the resulting dissertation and manuscripts will be submitted to the ARO archives.
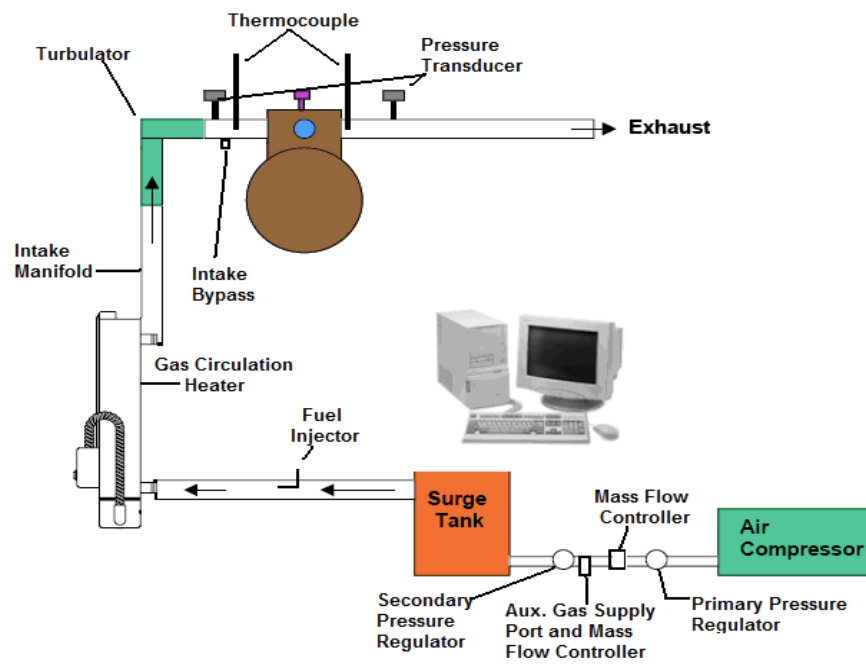
Figure 1. Schematic diagram of the single cylinder engine test facility used in this study.
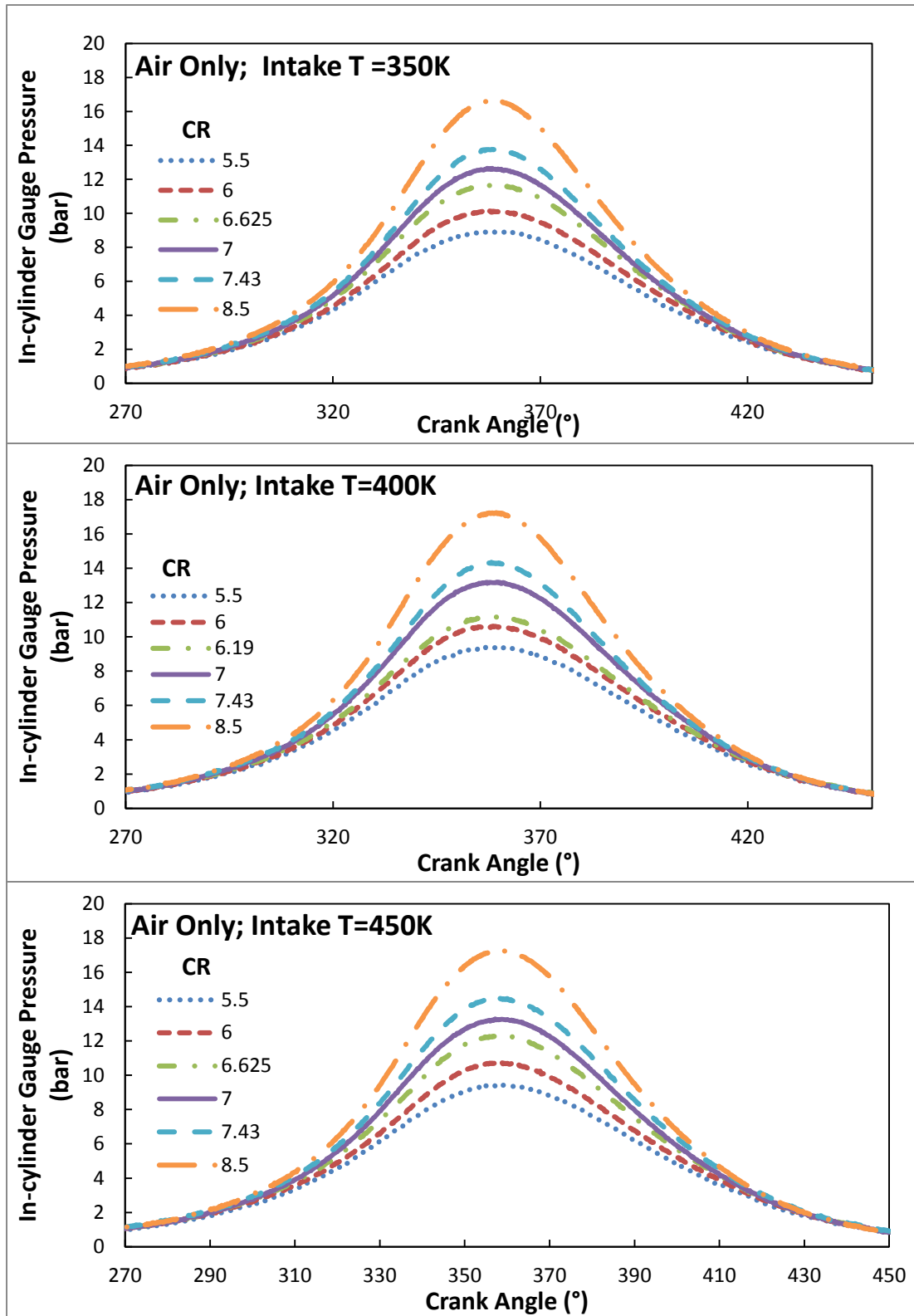
Figure 2. In-cylinder pressure profiles for an air charge for a range of intake temperatures and compression ratios.
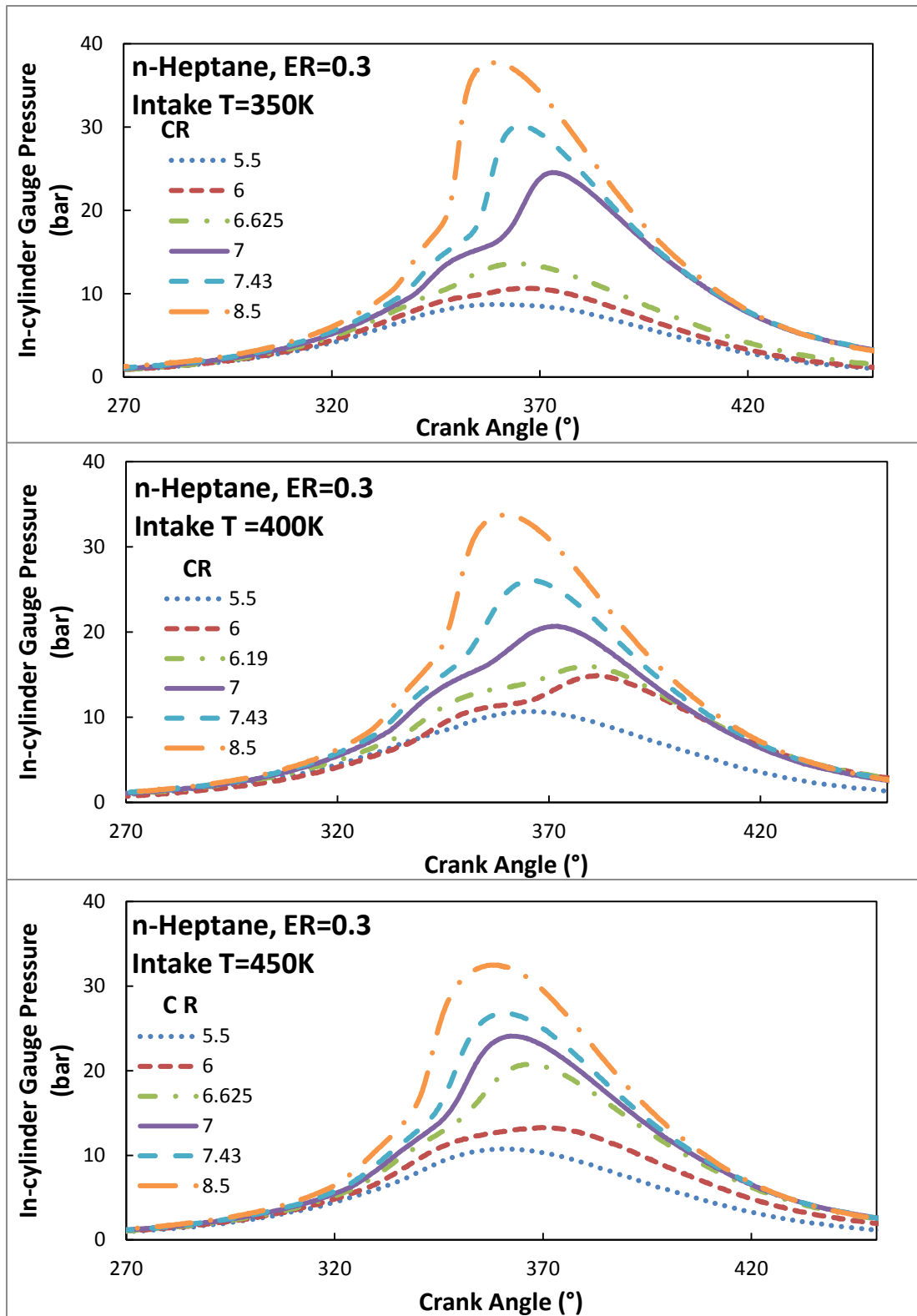
Figure 3. In-cylinder pressure profiles for n-heptane oxidation at ER=0.3 for three intake temperatures varying CR.
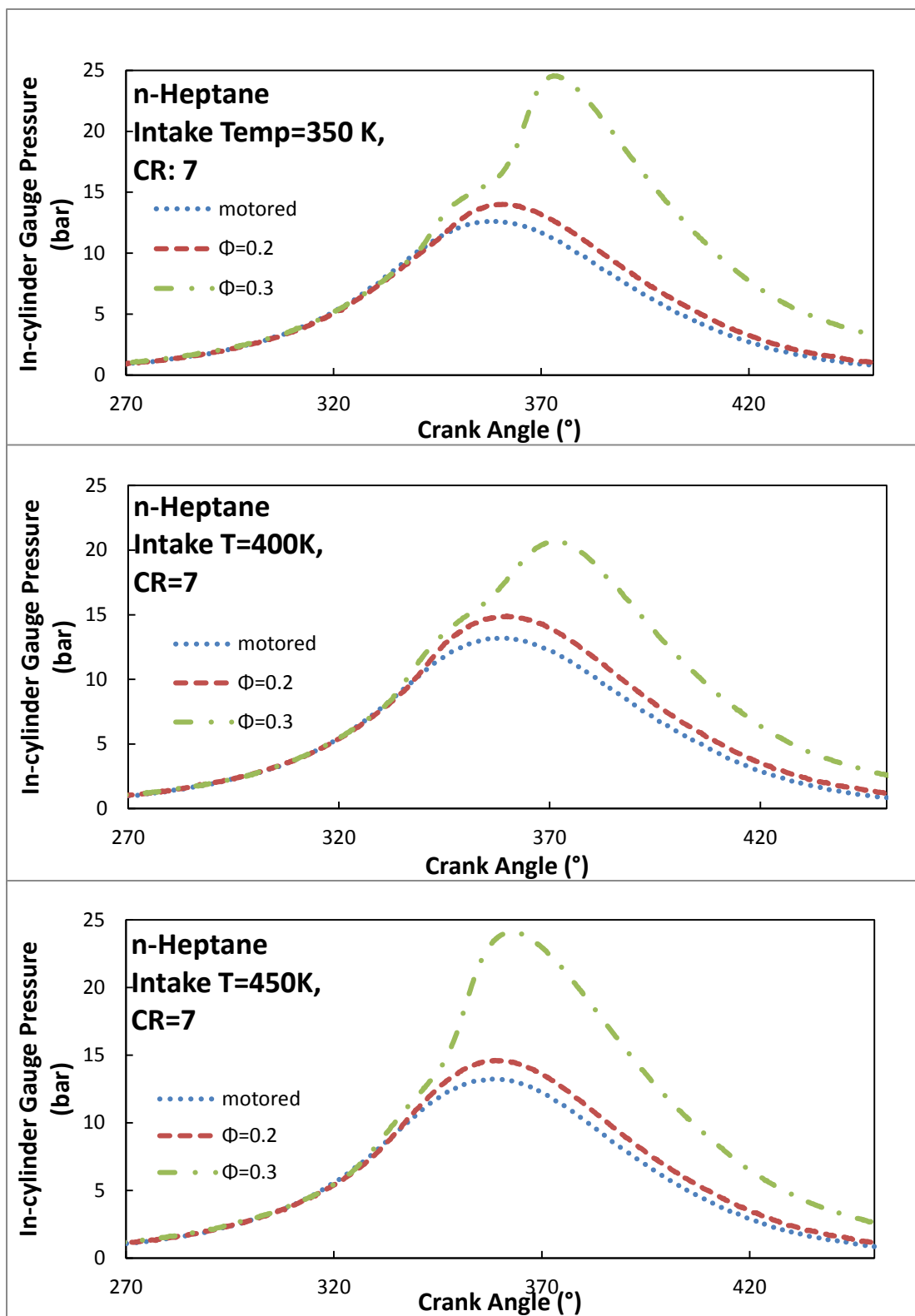
Figure 4. In-cylinder pressure profiles for n-heptane oxidation at CR=7 for three intake temperatures and and two ERs.

Figure 5. In-cylinder pressure profiles for n-heptane oxidation at CR=8.5 for three intake temperatures and two ERs.
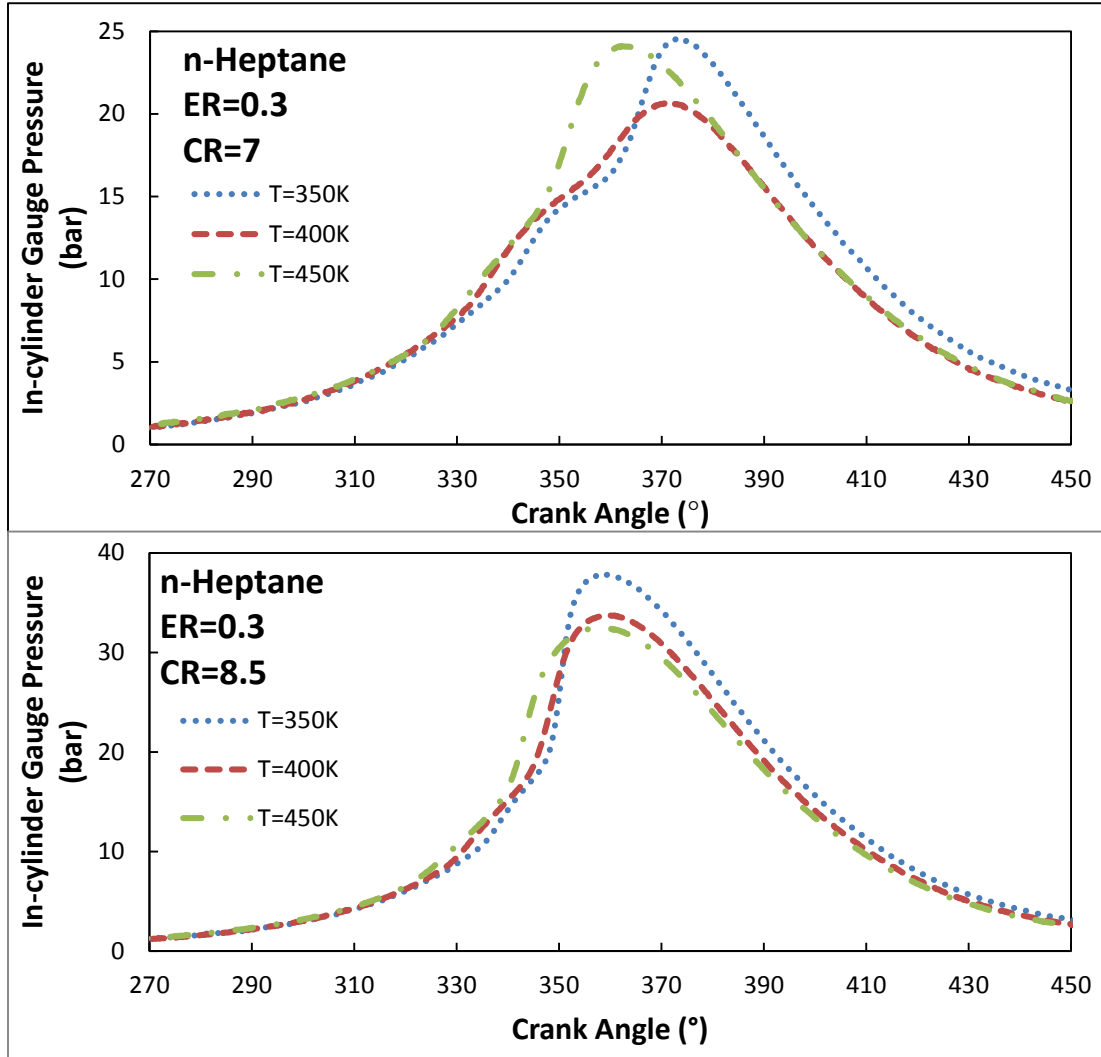
Figure 6. In-cylinder pressure profiles for n-heptane oxidation with ER=0.3, two CRs and three intake temperatures.
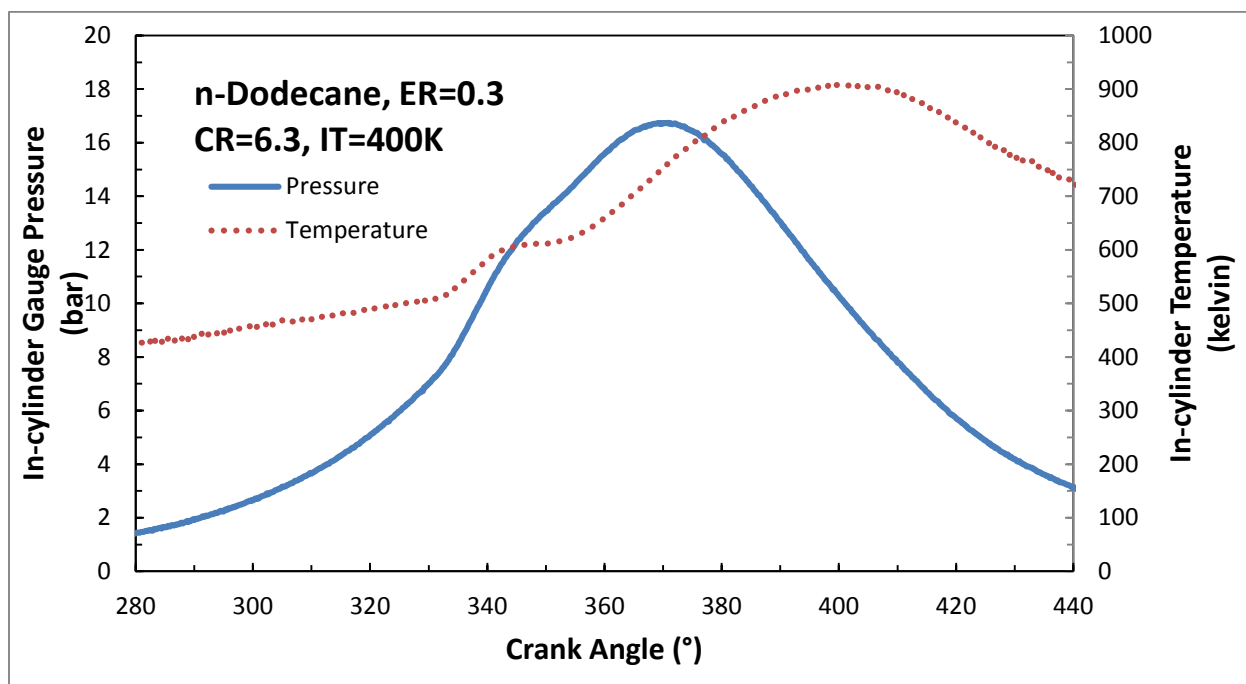
Figure 7. In-cylinder pressure and temperature profiles for n-dodecane oxidation at condition of ER=0.3, CR=6.3, IT=400K.
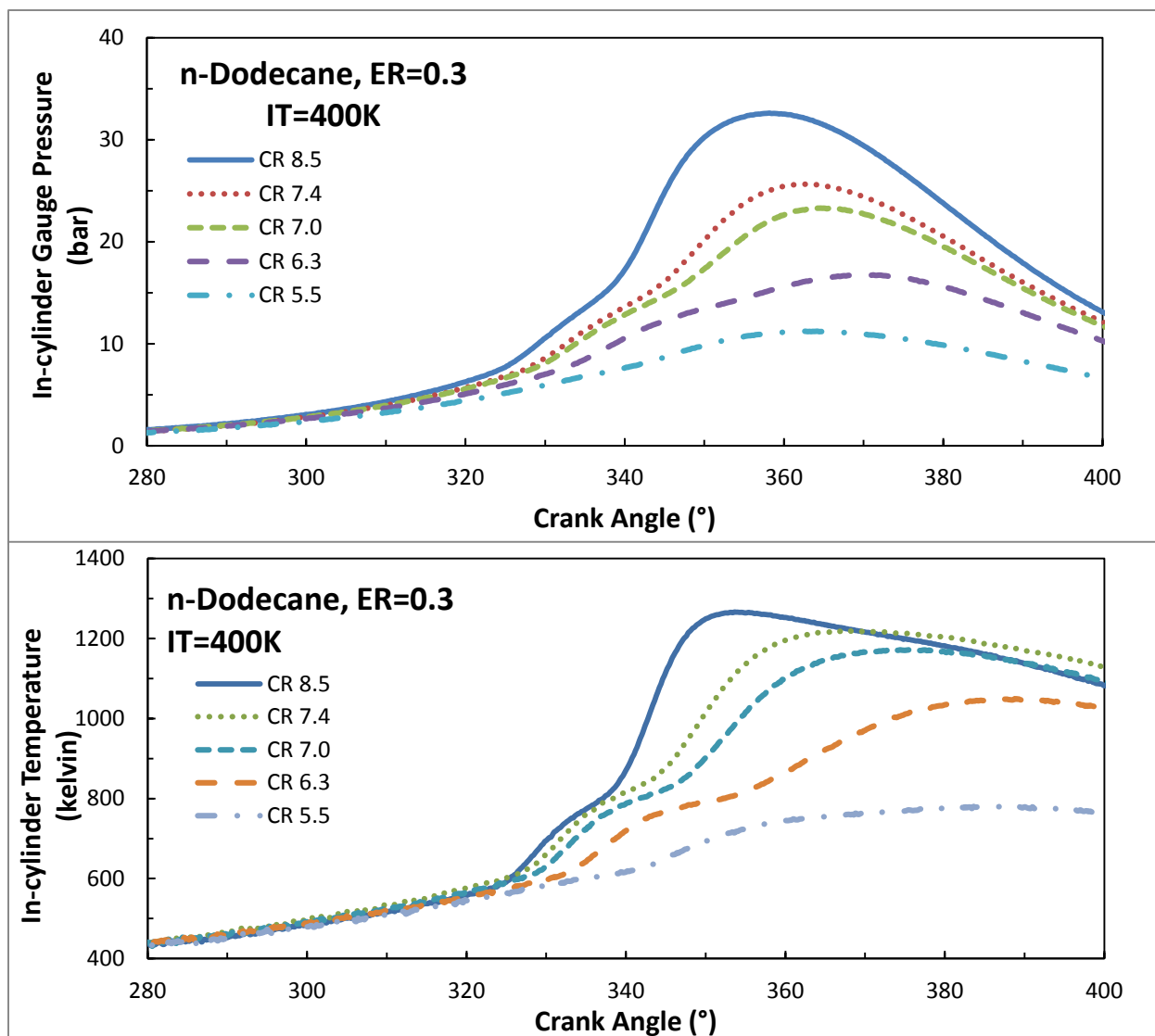
Figure 8. In-cylinder pressure and temperature profile for n-dodecane oxidation at condition of ER=0.3, IT=400K varying CR.
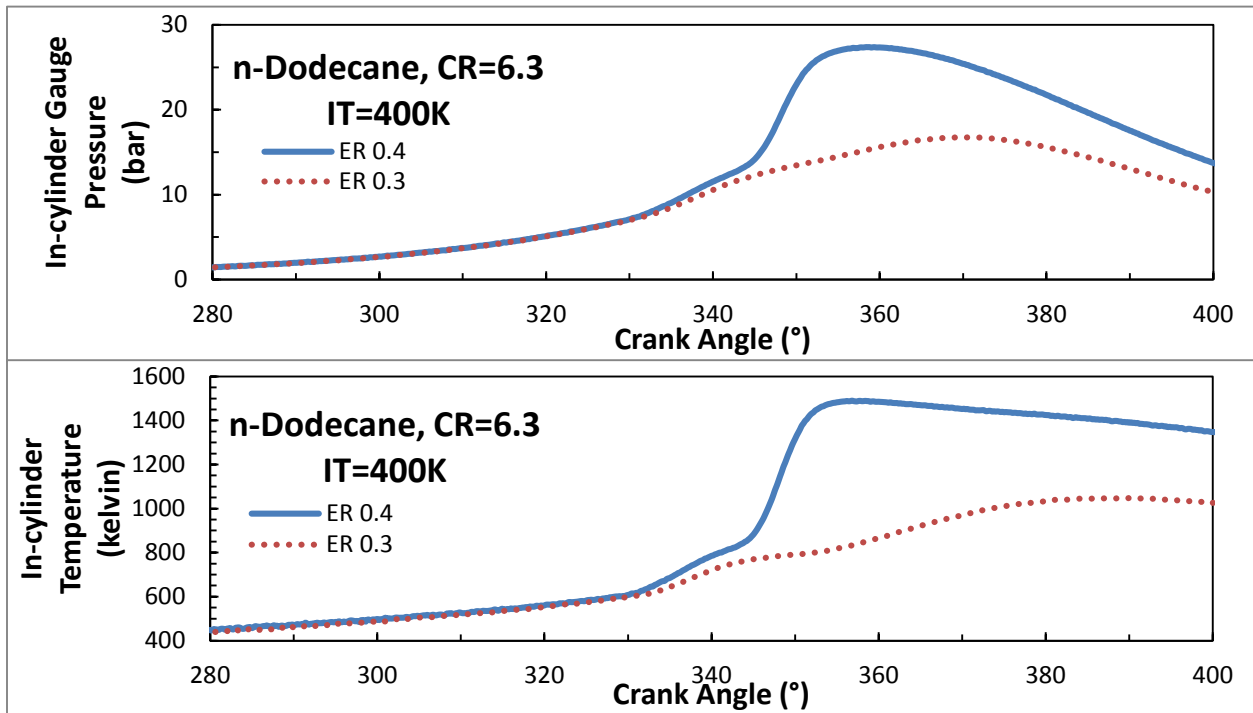
Figure 9. In-cylinder pressure and temperature profile for n-dodecane oxidation at condition of CR=6.3, IT=400K varying ER.
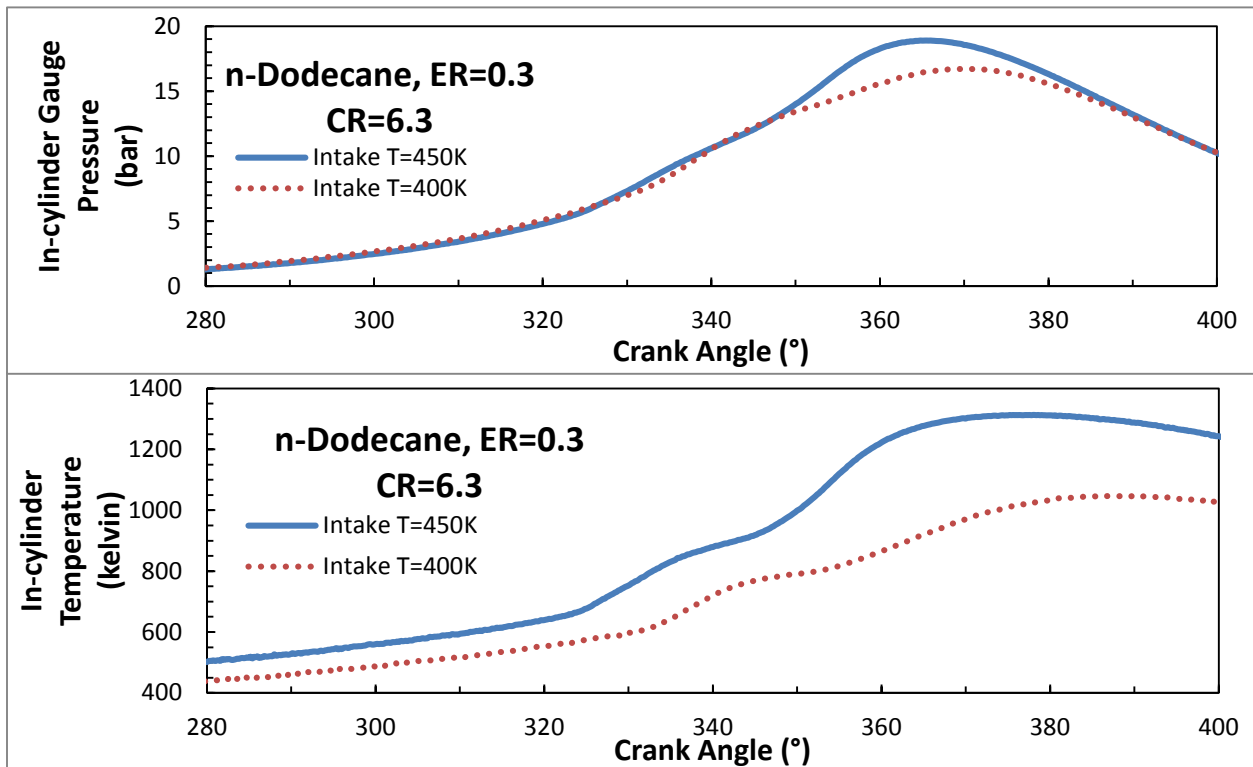
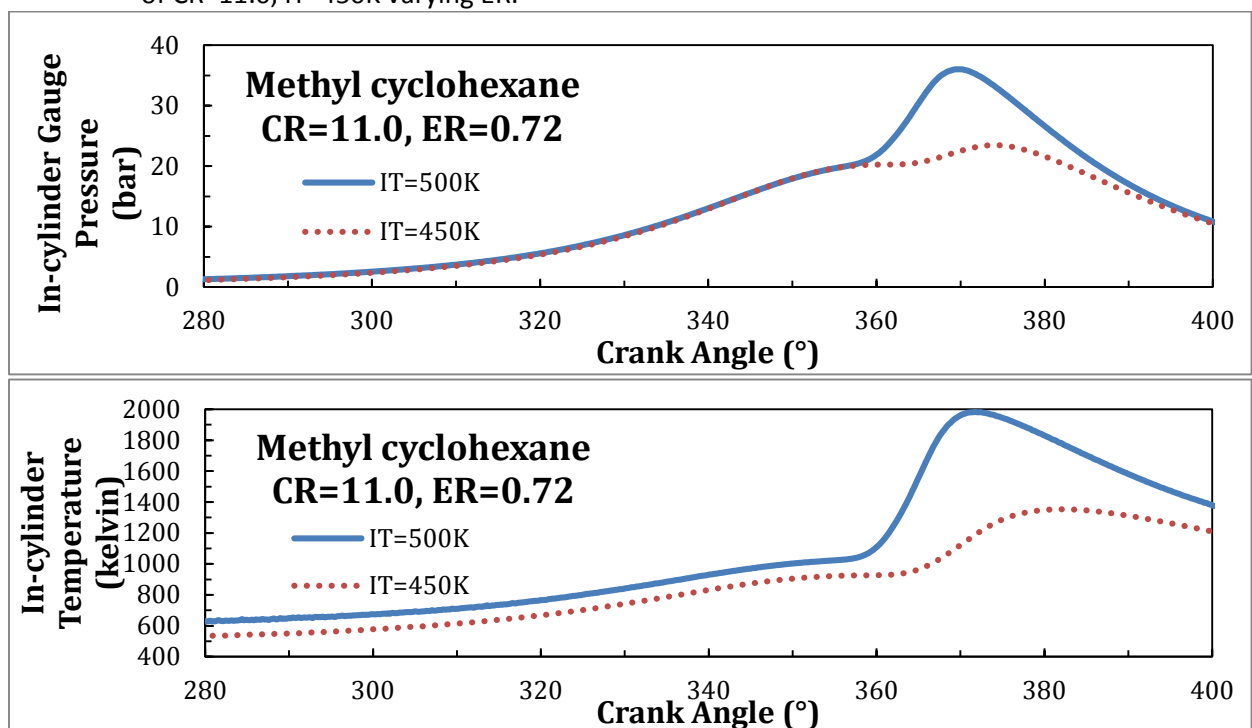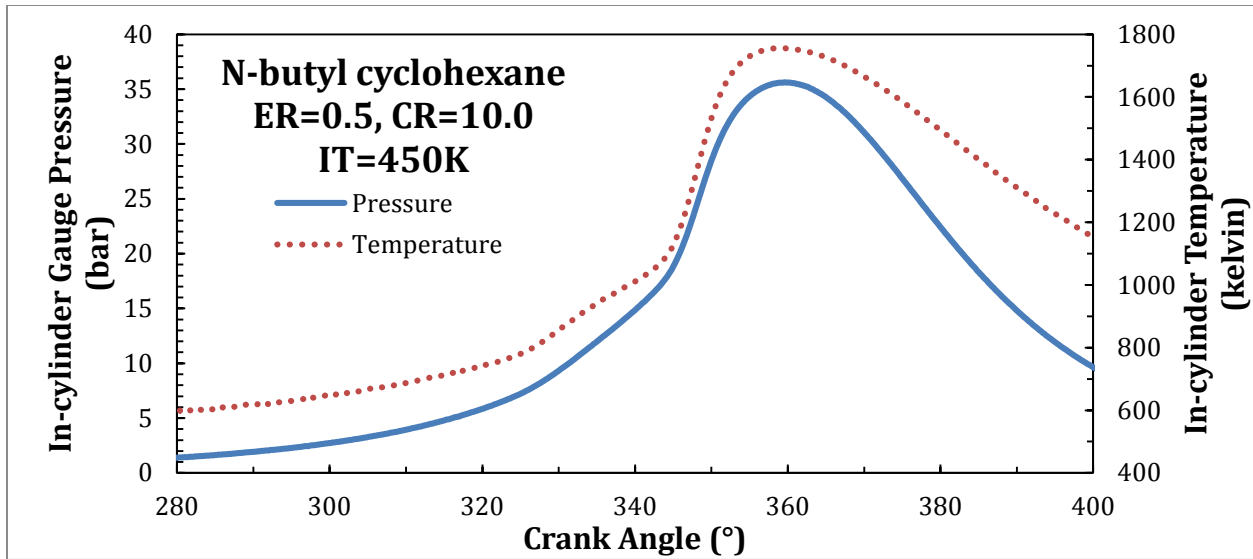Figure 10. In-cylinder pressure and temperature profile for n-dodecane oxidation at condition of ER=0.3 CR=6.3 varying IT.
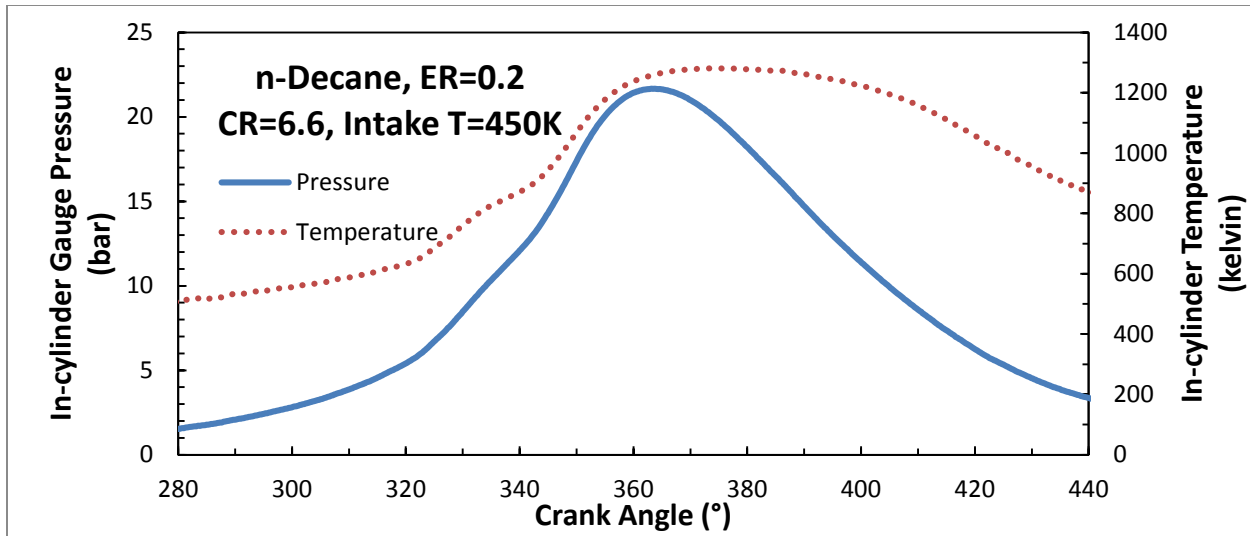
Figure 11. In-cylinder pressure and temperature profiles for n-decane oxidation at condition of ER=0.3, CR=6.3, IT=400K.
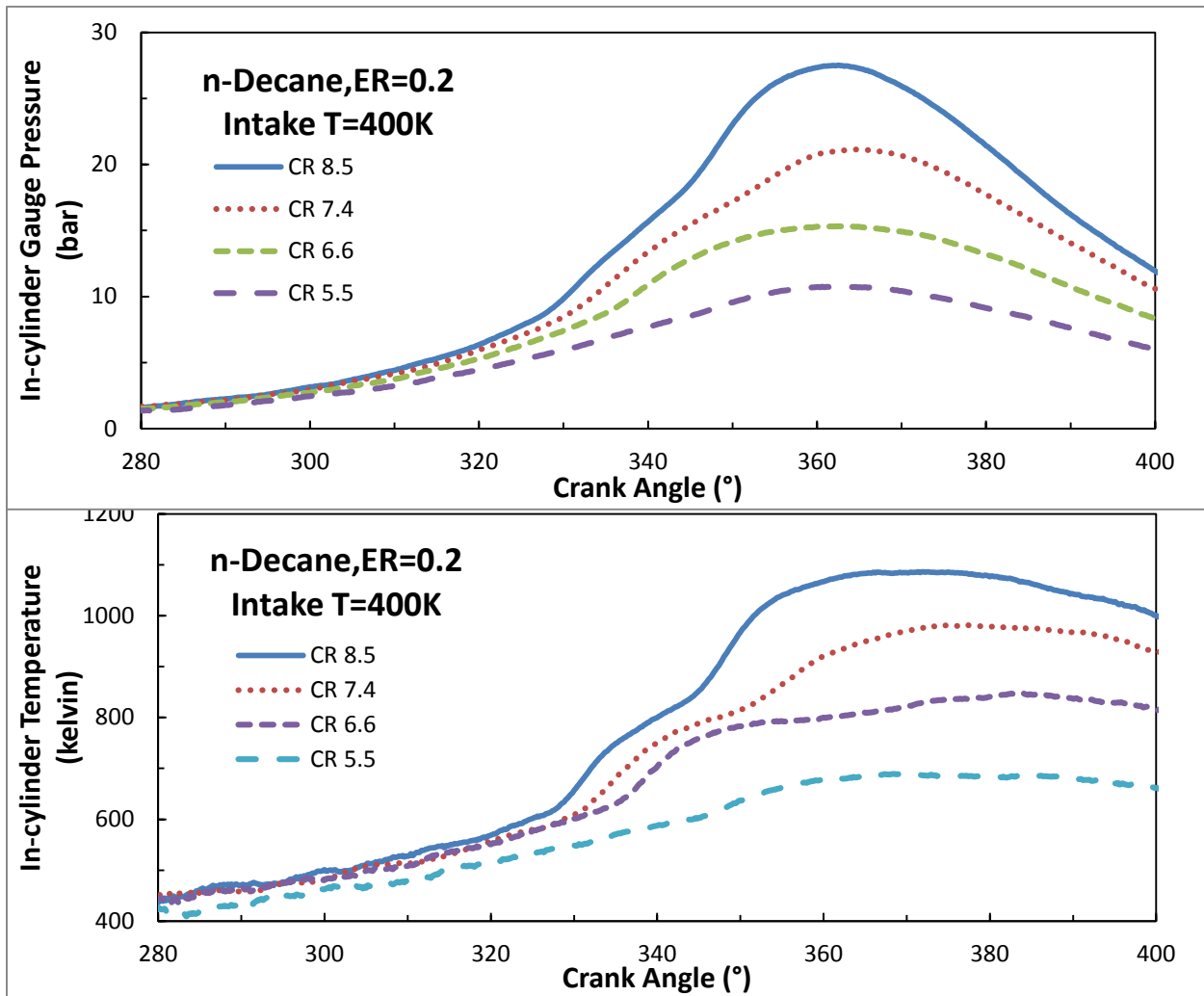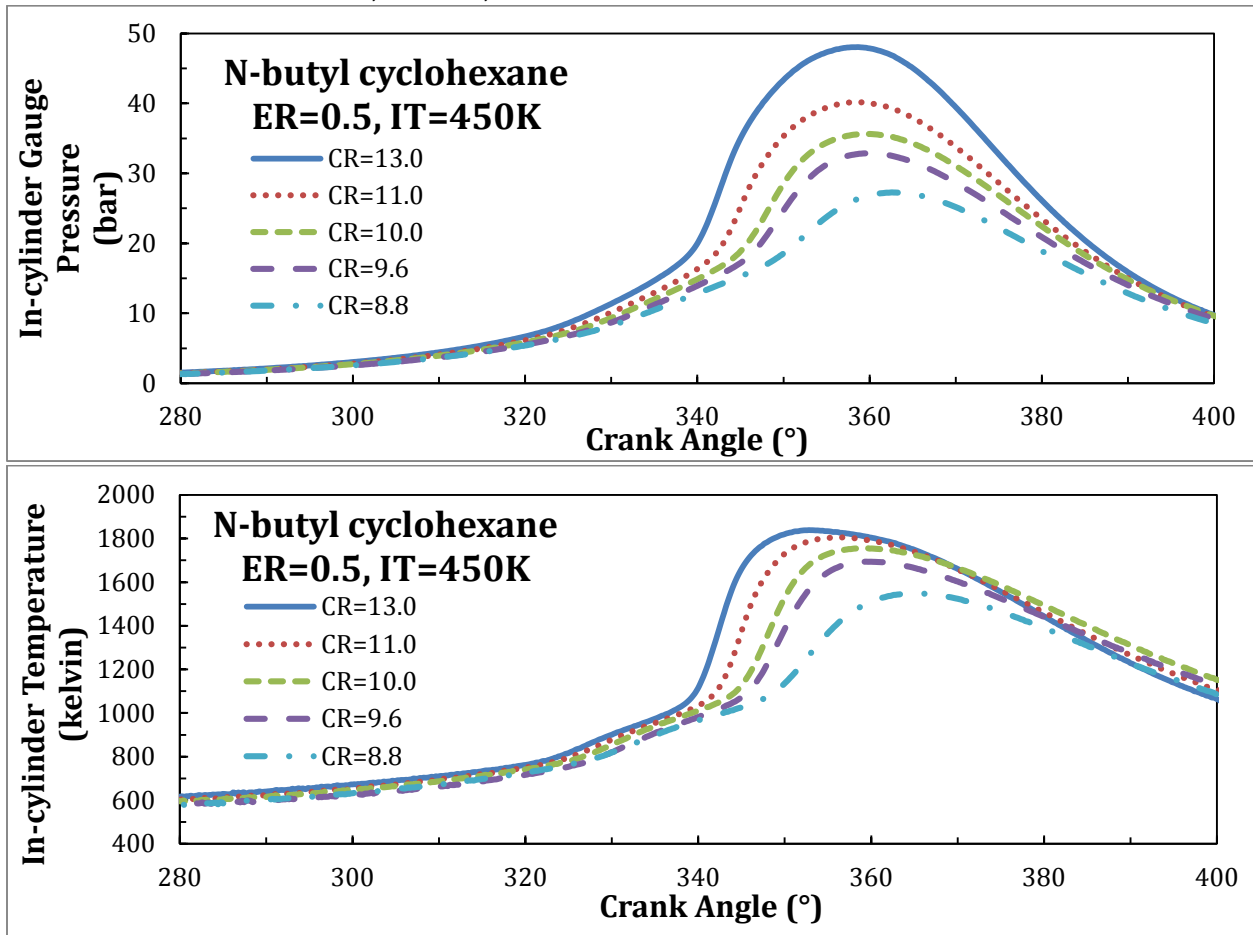

Figure 12. In-cylinder pressure and temperature profile for n-decane oxidation at condition of ER=0.2, IT= 400K varying CR.
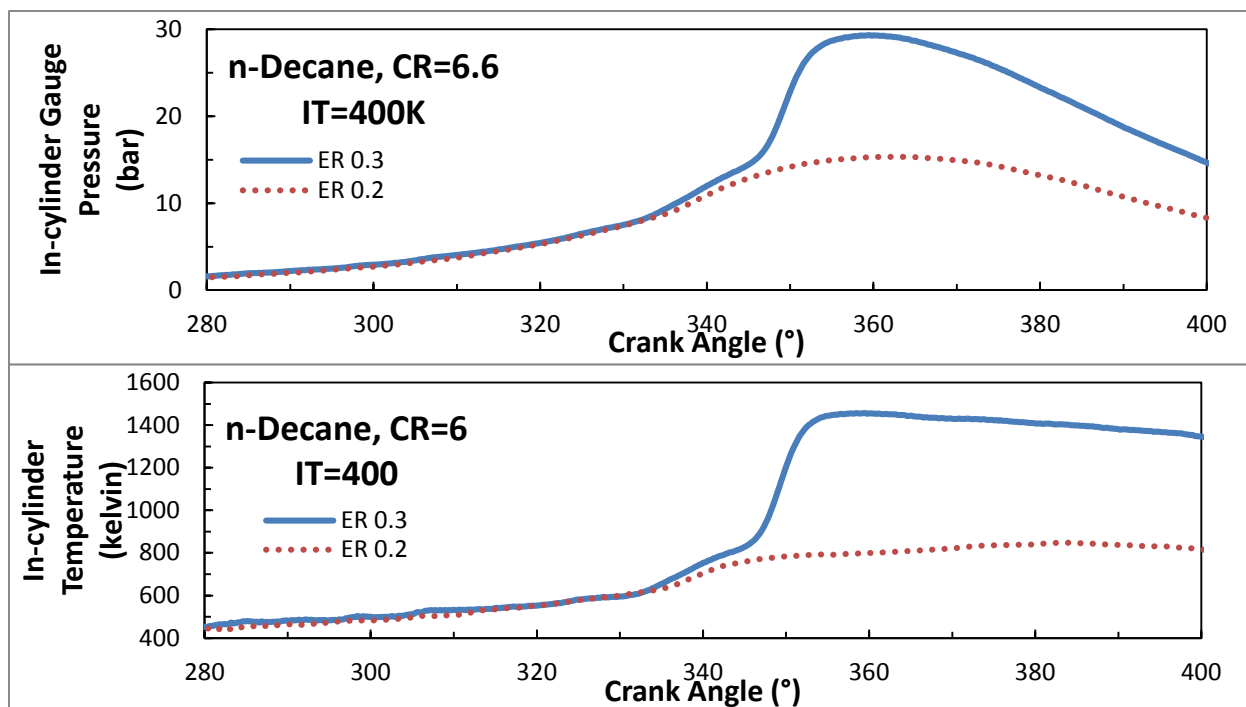
Figure 13. In-cylinder pressure and temperature profile for n-decane oxidation at condition of CR=6.6, IT= 400K varying ER.
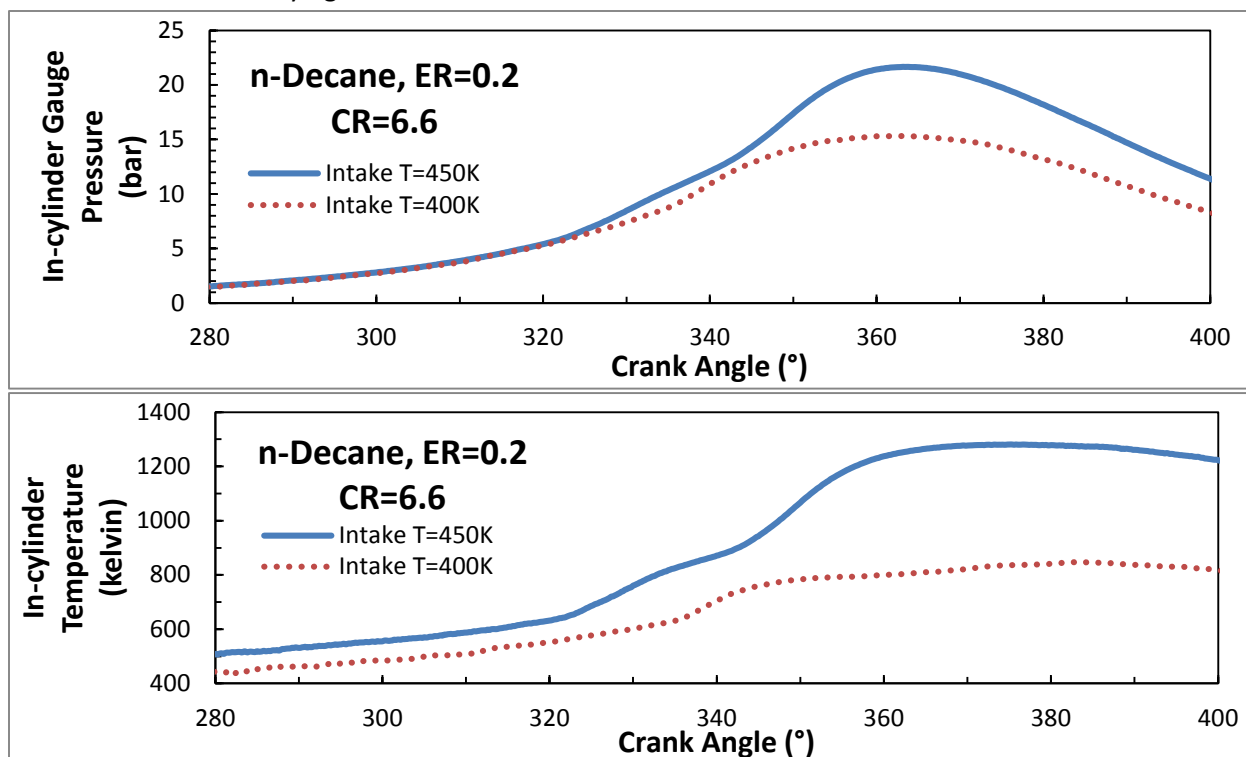
Figure 14. In-cylinder pressure and temperature profile for n-decane oxidation at condition of ER=0.2 CR=6.6 varying IT.
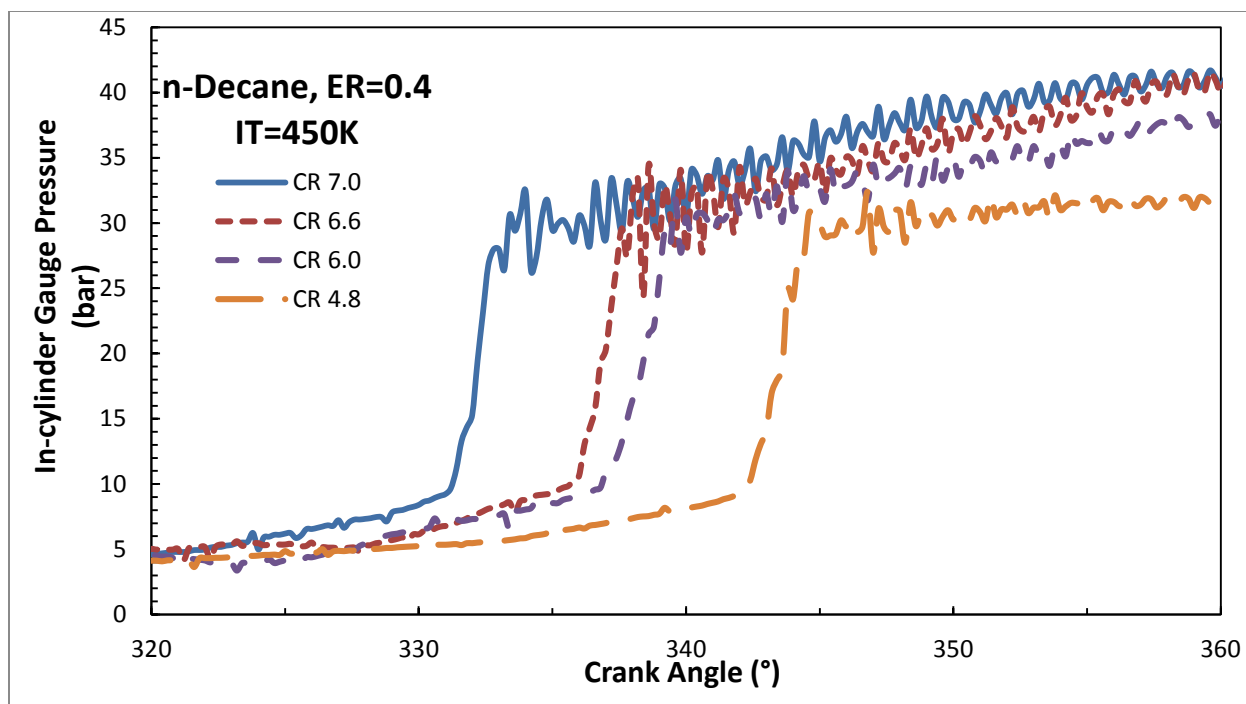
Figure 15. In-cylinder pressure profiles for n-decane oxidation at knocking condition.
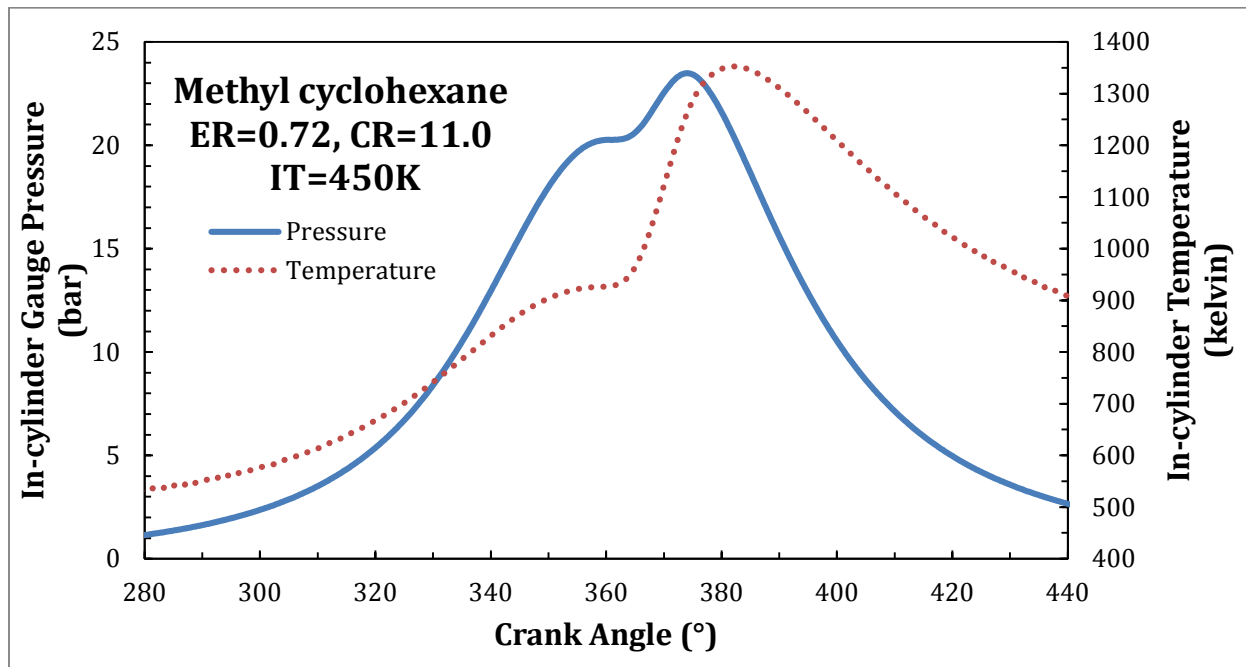
Figure 16. In-cylinder pressure and temperature profiles for methyl cyclohexane oxidation at condition of ER=0.72, CR=11.0, IT=450K.
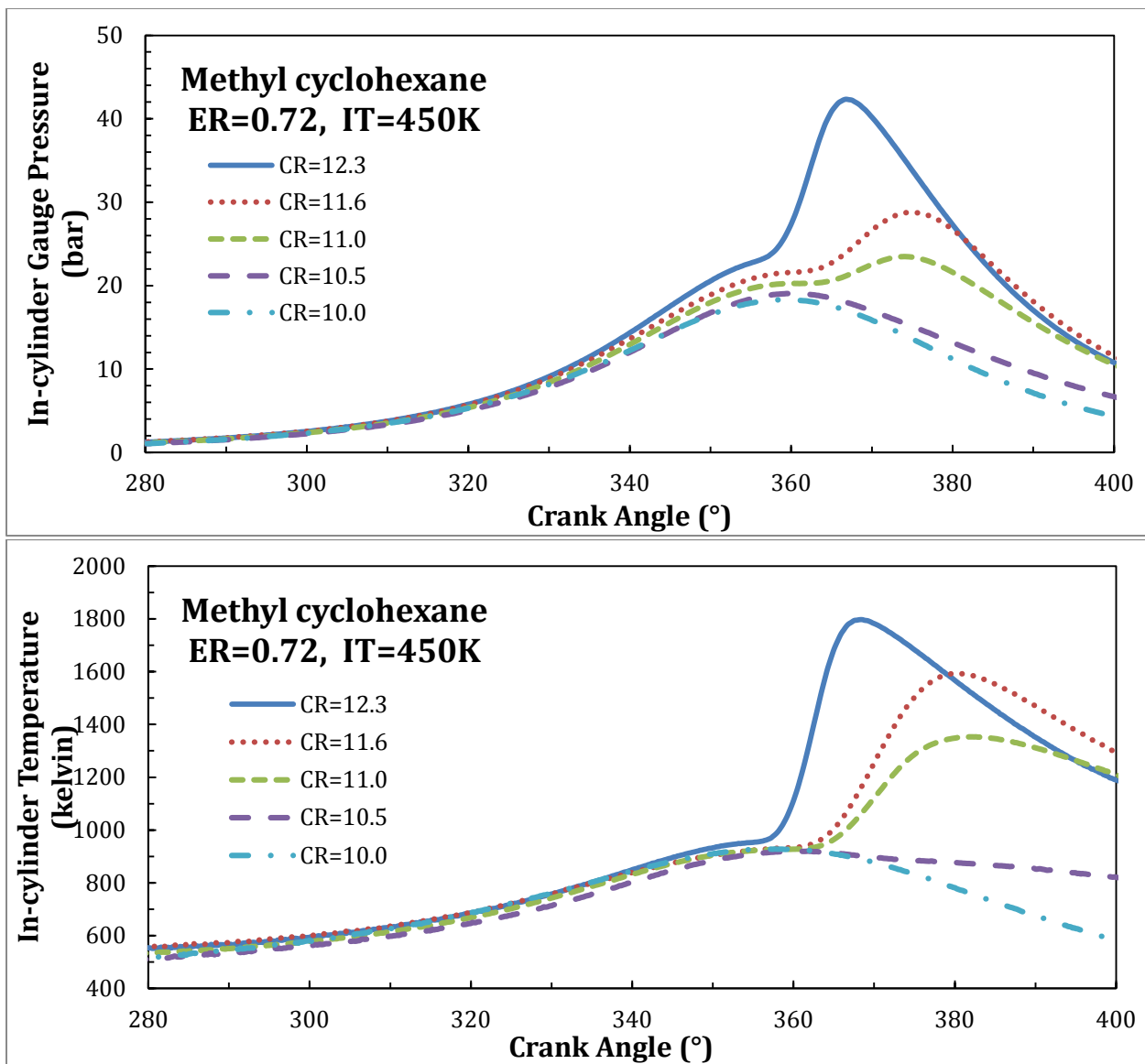
Figure 17. In-cylinder pressure and temperature profile for methyl cyclohexane oxidation at condition of ER=0.72, IT=450K varying CR.
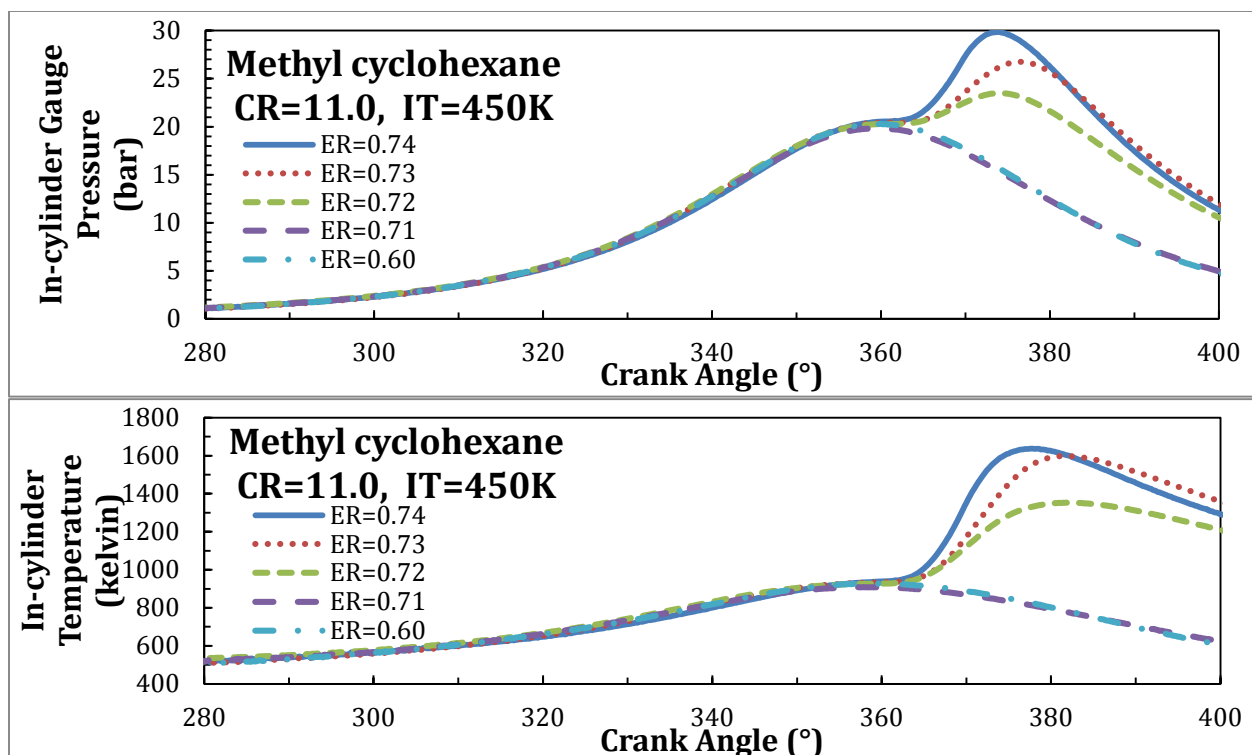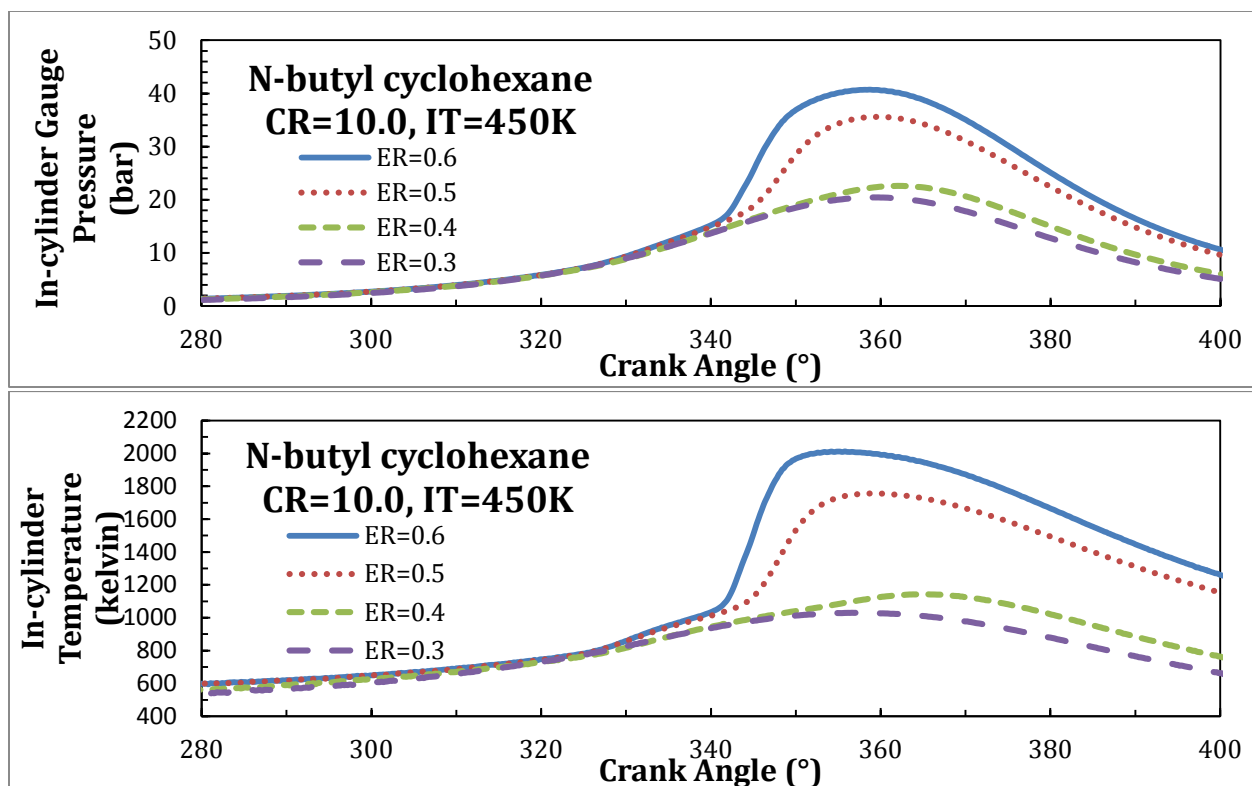
Figure 18. In-cylinder pressure and temperature profile for methyl cyclohexane oxidation at condition of CR=11.0, IT=450K varying ER.
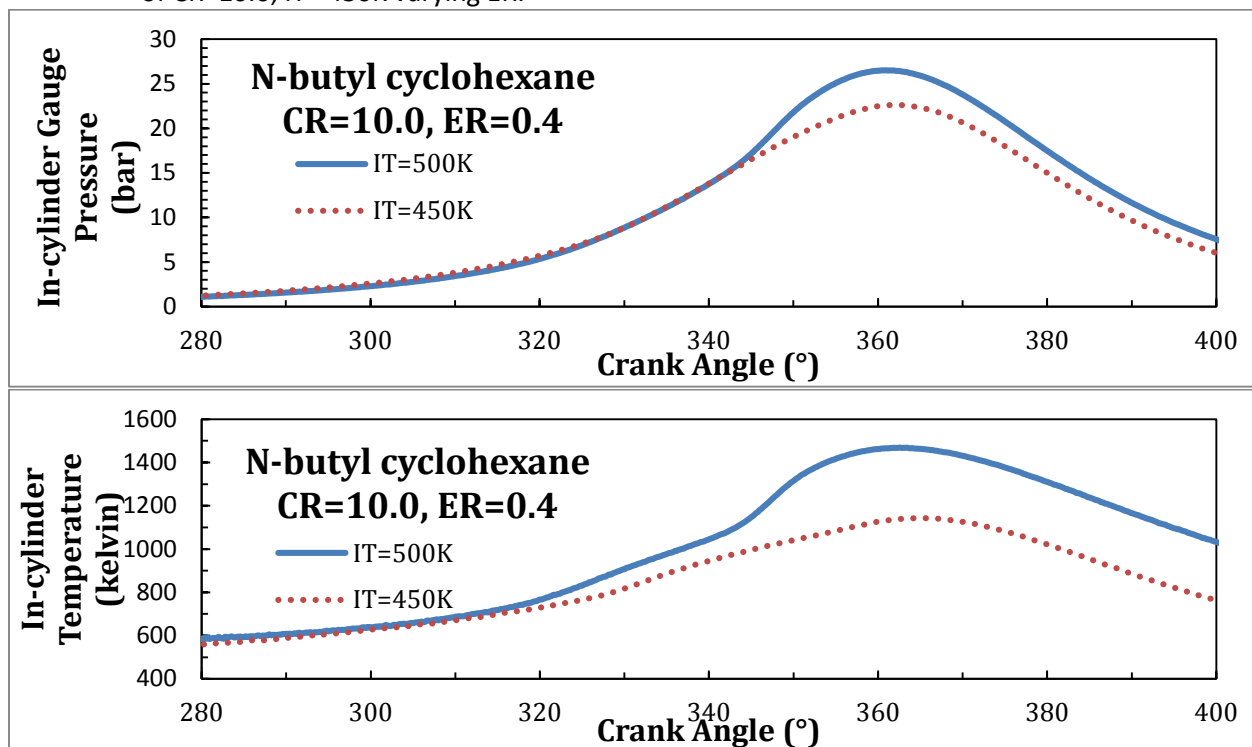

Figure 19. In-cylinder pressure and temperature profile for methyl cyclohexane oxidation at condition of CR=11.0, ER=0.72 varying IT.
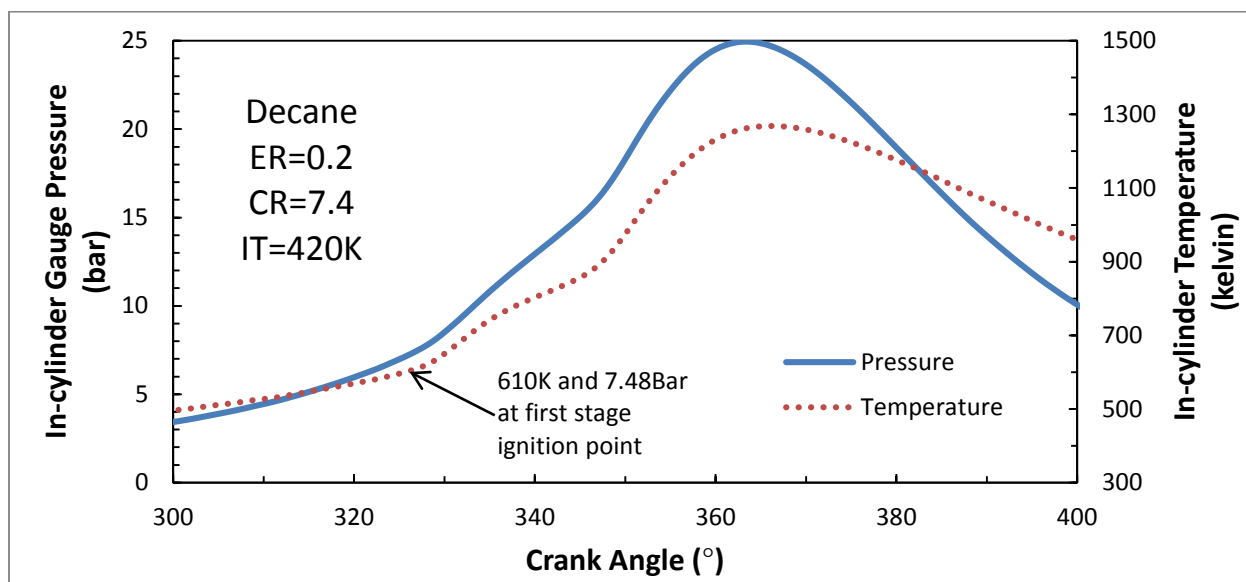
21

Figure 20. In-cylinder pressure and temperature profiles for n-butyl cyclohexane oxidation at condition of ER=0.5, CR=10.0, IT=450K.

Figure 21. In-cylinder pressure and temperature profile for n-butyl cyclohexane oxidation at condition of ER=0.5, IT= 450K varying CR

Figure 22. In-cylinder pressure and temperature profile for n-butyl cyclohexane oxidation at condition of CR=10.0, IT= 450K varying ER.

Figure 23. In-cylinder pressure and temperature profile for n-butyl cyclohexane oxidation at condition of ER=0.4 CR=10.0 varying IT.
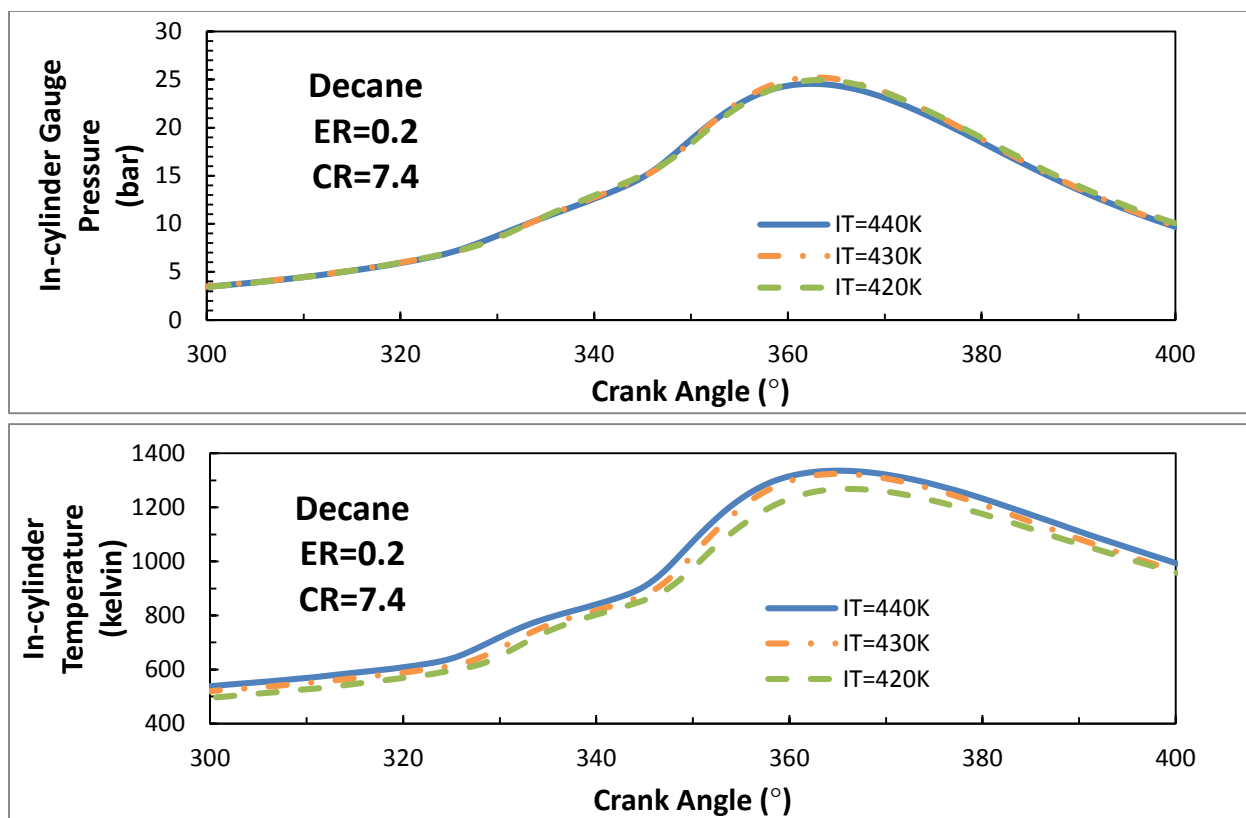
Figure 24.　In-cylinder pressure and temperature profiles for decane oxidation at condition of ER=0.2, CR=7.4, IT=420K.
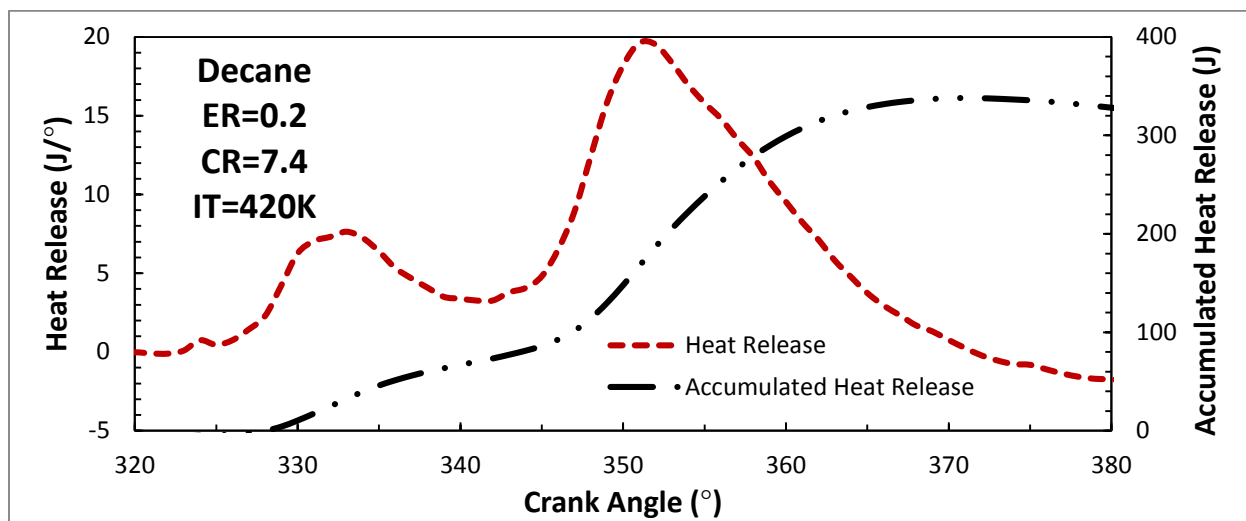
Figure 25.　Heat release per degree and accumulated heat release profiles for decane oxidation at condition of ER=0.2, CR=7.4, IT=420K.

Figure 26. In-cylinder pressure and temperature profiles for decane oxidation at condition of ER=0.2, CR=7.4 varying IT.
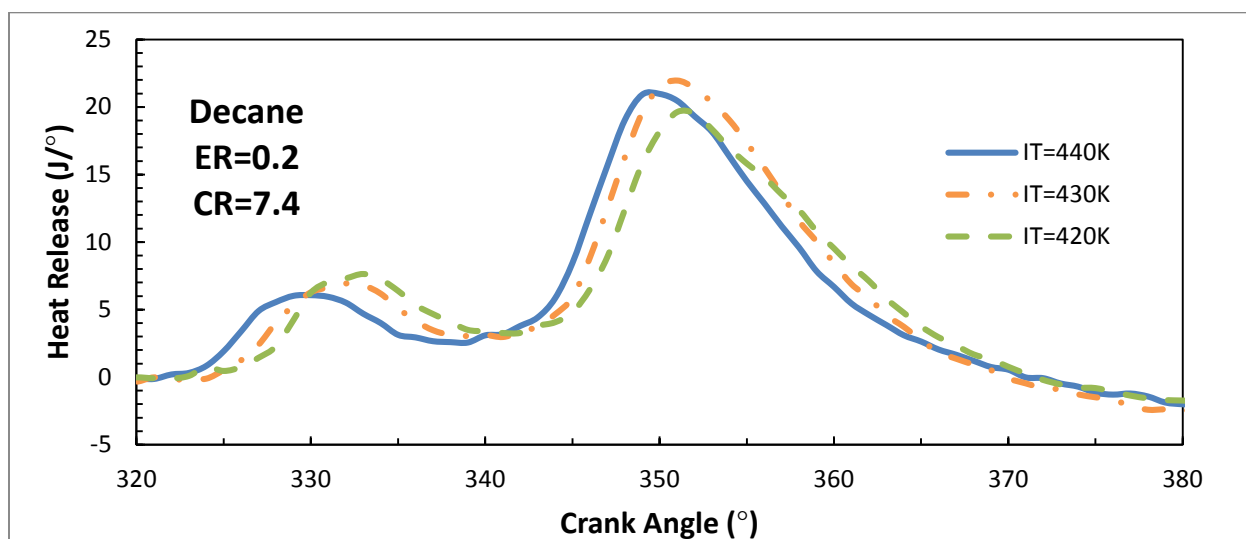

Figure 27. Heat release profiles for decane oxidation at condition of ER=0.2, CR=7.4 varying IT.
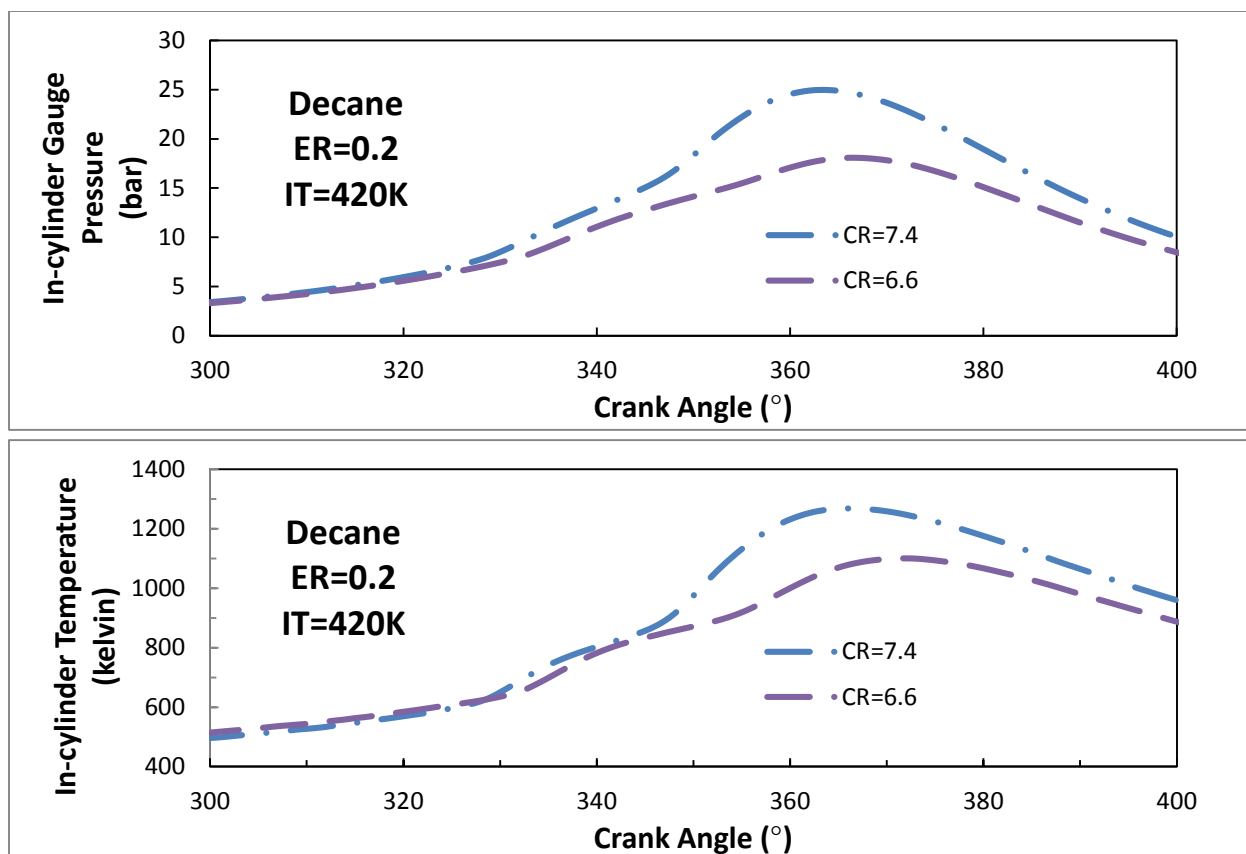
Figure 28. In-cylinder pressure and temperature profiles for decane oxidation at condition of ER=0.2, IT=420K varying CR.
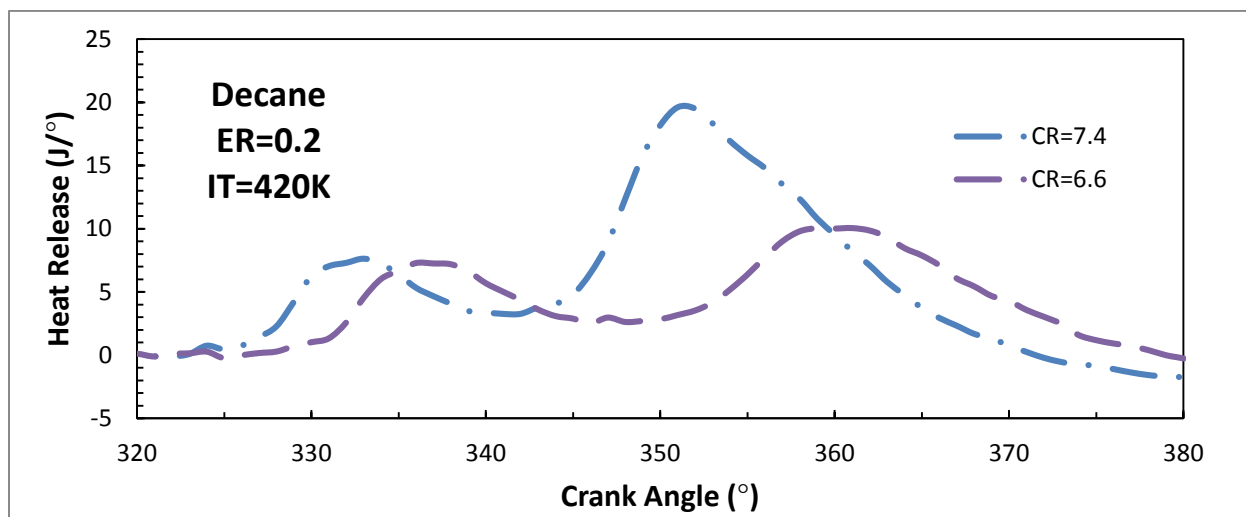

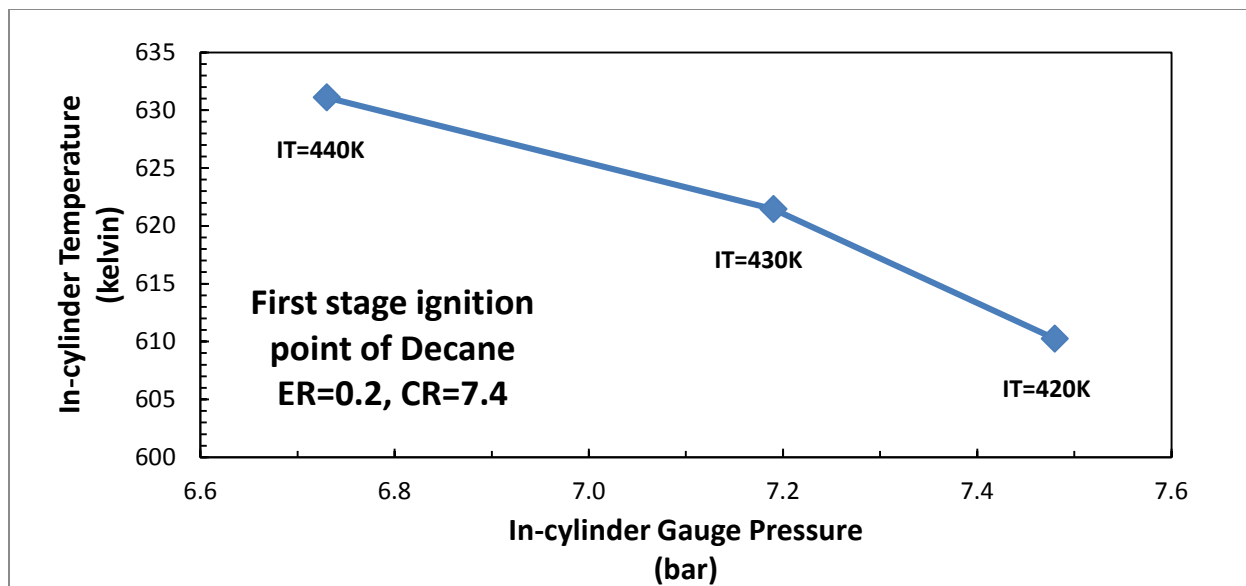Figure 29. Heat release profiles for decane oxidation at condition of ER=0.2, IT=420K varying CR.

Figure 30.   Pressure and temperature at first stage ignition point with different ITs.